- 1 APPENDIX 1
- 2 Andrea, T.A., et al. J Med Chem 22, 221-232 (1979).
- 3 Andrews et al, U.S. Patent No. 4,741,897, issued May 3, 1989.
- 4 Apriletti, J.W., Baxter, J.D., Lau, K.H & West, B.L. Protein Expression and
- 5 Purification 6, 363-370 (1995).
- 6 Apriletti, J.W., Baxter, J.D. & Lavin, T.N. J. Biol. Chem. 263, 9409-9417 (1988).
- Au-Fliegner, M., Helmer, E., Casanova, J., Raaka, B.M. & Samuels, H.H. Mol Cell
- 8 *Biol* 13, 5725-5737 (1993).
- 9 Baniahmad, A., et al. Mol Cell Biol 15, 76-86 (1995).
- Barettino, D., Vivanco Ruiz, M.M. & Stunnenberg, H.G. Embo J 13, 3039-3049
- 11 (1994).
- 12 Beck-Peccoz, P., et al. J Clin Endocrinol Metab 78, 990-993 (1994).
- Bhat, M.K., McPhie, P. & Cheng, S.Y. Biochem Biophys Res Commun 210, 464-471
- 14 (1995).
- 15 Blake, C.C. & Oatley, S.J. Nature 268, 115-120 (1977).
- 16 Blake, C.C., Geisow, M.J., Oatley, S.J., Rerat, B. & Rerat, C. J Mol Biol 121, 339-
- 17 356 (1978).
- Bourguet, W., Ruff, M., Chambon, P., Gronemeyer, H. & Moras, D. Nature 375,
- 19 377-382 (1995).
- 20 Brent, G.A. N Engl J Med 331, 847-853 (1994).
- 21 Brunger, A.T., Kuriyan, J. & Karplus, M. Science 235, 458-460 (1987).
- 22 Casanova, J., et al. Mol Cell Biol 14, 5756-5765 (1994).
- 23 Cavailles, V., et al. Embo J 14, 3741-3751 (1995).

- 1 Chin et al, U.S. Patent No. 5,284,999, issued February 8, 1994.
- 2 Collaborative Computational Project, N.4. Acta Crystallogr. **D50**, 760-763 (1994).
- Collingwood, T.N., Adams, M., Tone, Y & Chatterjee, V.K. Mol Endocrinol 8.
- 4 1262-1277 (1994).
- 5 Cowtan, K. Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography 31.
- 6 34-38 (1994).
- 7 Damm, K. & Evans, R.M. Proc Natl Acad Sci U S A 90, 10668-10672 (1993).
- 8 Danielian, P.S., White, R., Lees, J.A. & Parker, M.G. Embo J 11, 1025-1033
- 9 (1992).
- Davies et al, U.S. Patent No. 5,322,933, issued June 21, 1994.
- Dawson et al, U.S. Patent No. 5,466,861, issued November 14, 1995.
- DeGroot et al, U.S. Patent No. 5,438,126, issued August 1, 1995.
- Dietrich, S.W., Bolger, M.B., Kollman, P.A. & Jorgensen, E.C. J Med Chem 20,
- 14 863-880 (1977).
- 15 Durand, B., et al. Embo J 13, 5370-5382 (1994).
- 16 Ellis et al, U.S. Patent No. 4,766,121, issued August 23, 1988.
- 17 Ellis et al, U.S. Patent No. 4,826,876, issued May 2, 1989.
- 18 Ellis et al, U.S. Patent No. 4,910,305, issued March 20, 1990.
- 19 Emmett et al, U.S. Patent No. 5,061,798, issued October 29, 1991.
- 20 Evans, R.M. Science 240, 889-895 (1988).
- 21 Evans et al, U.S. Patent No. 5,171,671, issued December 15, 1992.
- 22 Evans et al, U.S. Patent No. 5,312,732, issued May 17, 1994.
- 23 Fawell, S.E., Lees, J.A., White, R. & Parker, M.G. Cell 60, 953-962 (1990).

- 1 Forman, B.M. & Samuels, H.H. Mol. Endocrinol. 4, 1293-1301 (1990).
- Gewirth, D.T. & Sigler, P.B. Nature Structural Biology 2, 386-394 (1995).
- Glass, C.K. Endocr Rev 15, 391-407 (1994).
- 4 Hayashi, Y. Sunthornthepvarakul, T. & Refetoff, S. J Clin Invest 94, 607-615
- 5 (1994).
- Jones, T.A., Zou, J.Y., Cowan, S.W. & Kjeldgaard. Acta Crystallogr A 47, 110-119
- 7 (1991).
- 8 Jorgensen, E.C. in Hormonal Peptides and Proteins (eds. Li, C.H.) 107-204
- 9 (Academic Press, New York, 1978).
- 10 Kabsch, W. J. Appl. Crystallogr. 26, 795-800 (1993).
- 11 Kabsch, W. & Sander, C. Biopolymers 22, 2577-2637 (1983).
- 12 Laskowski, R.A., Macarthur, M.W., Moss, D.S. & Thornton, J.M. J. Appl.
- 13 Crystallogr. 26, 283-291 (1993).
- Latham, K.R., Apriletti, J.W., Eberhardt, N.L. & Baxter, J.D. J Biol Chem 256,
- 15 12088-12093 (1981).
- 16 Laudet, V., Hanni, C., Coll, J., Catzeflis, F. & Stehelin, D. Embo J 11, 1003-1013
- 17 (1992).
- 18 LeDouarin, B., et al. Embo J 14, 2020-2033 (1995).
- Lee, J.W., Ryan, F., Swaffield, J.C., Johnston, S.A. & Moore, D.D. Nature 374,
- 20 91-94 (1995).
- Lee, J.W., Choi, H.S., Gyuris, J., Brent, R. & Moore, D.D. Molec. Endocrinol. 9,
- 22 243-254 (1995).

- 1 Leeson, P.D., Emmett, J.C., Shah, V.P., Showell, G.A., Novelli, R., Prain, H.D.,
- Benson, M.G., Ellis, D., Pearce, N.J. & Underwood, A.H. J. Med. Chem. 32, 320-
- 3 336 (1989).
- Leeson, P.D., Ellis, D., Emmett, J.D., Shah, V.P., Showell, G.A. & Underwood,
- 5 A.H. J. Leng, X., et al. Mol Cell Biol 15, 255-263 (1995).
- Leng, X., Tsai, S.Y., O'Malley, B.W. & Tsai, M.J. J Steroid Biochem Mol Biol 46,
- 7 . 643-661 (1993).
- 8 Lin, K.H., Parkison, C., McPhie, P. & Cheng, S.Y. Mol. Endocrinol. 5, 485-492
- 9 (1991).
- 10 Luisi, B.F., et al. Nature 352, 497-505 (1991).
- 11 McGrath, M.E., et al. J. Mol. Biol. 237, 236-239 (1994).
- McRee, D.E., Practical Protein Crystallography, Academic Press, N.Y. (1993),
- especially chapters 1, 2 and 3.
- 14 Meier, C.A., et al. Mol. Endocrinol. 6, 248-258 (1992).
- 15 Miura et al, U.S. Patent No. 5,116,828, issued May 26, 1992.
- 16 Monaco, H.L., Rizzi, M. & Coda, A. Science 268, 1039-1041 (1995).
- 17 Nicholls, A., Sharp, K.A. & Honig, B. *Proteins* 11, 281-296 (1991).
- O'Donnell, A.L., Rosen, E.D., Darling, D.S. & Koenig, R.J. Mol. Endocrinol. 5,
- 19 94-99 (1991).
- 20 Otwinowski, Z. Proceedings of the CCP4 Study Weekend 80-86 (SERC Daresbury
- 21 Laboratory, Warrington, U.K., 1991).
- 22 Otwinowski, Z. Proceedings of the CCP4 Study Weekend: "Data Collection and
- 23 Processing 56-62 (SERC Daresbury Laboratory, Warrington, U.K., 1993).

- Ozato, U.S. Patent No. 5,403,925, issued April 4, 1995.
- Rastinejad, R., Perlmann, T., Evans, R.M. & Sigler, P.B. Nature 375, 203-211
- 3 (1995).
- 4 Refetoff, S., Weiss, R.E. & Usala, S.J. Endocr. Rev. 14, 348-399 (1993).
- 5 Ribeiro, R.C.J., Kushner, P.J. & Baxter, J.D. Annu. Rev. Med. 46, 443-453 (1995).
- 6 Ribeiro, R.C.J., et al. Ann. N. Y. Acad. Sci. 758, 366-389 (1995).
- Ribeiro, R.C., Kushner, P.J., Apriletti, J.W., West, B.L. & Baxter, J.D. Mol.
- 8 Endocrinol. 6, 1142-1152 (1992).
- 9 Saatcioglu, F., Bartunek, P., Deng, T., Zenke, M. & Karin, M. Mol. Cell Biol. 13,
- 10 3675-3685 (1993).
- 11 Schwabe, J.W., Chapman, L., Finch, J.T. & Rhodes, D. Cell 75, 567-578 (1993).
- 12 Selmi, S. & Samuels, H.H. J. Biol. Chem. 266, 11589-11593 (1991).
- 13 Swaffield, J.C., Melcher, K. & Johnston, S.A. Nature 374, 88-91 (1995).
- 14 Toney, J.H. et al. Biochemistry 32, 2-6 (1993).
- 15 Tsai, M.J. & O'Malley, B.W. Annu. Rev. Biochem. 63, 451-486 (1994).
- 16 Zenke, M., Munoz, A., Sap, J., Vennstrom, B. & Beug, H. Cell 61, 1035-1049
- 17 (1990).

APPENDIX 2 Table 8

3	Dimit	Amino Acid		
3 4 5 6 7 8 9	Atom	in full length a	Amino Acid Atom	<u>Distance</u>
5	C16			Α
6	C16	215-PHE	CD1	3.98
7	C19	215-PHE	CE1	3.86
é	C19	218-PHE	0	3.69
ő		218-PHE	СВ	3.89
10	C18 -	218-PHE	СВ	3.92
11	C19	218-PHE	СВ	4.13
11	C18	218-PHE	CD2	3.77
12	C16	219-THR	CG2	3.68
13	C19	221-ILE	CG1	4.11
14	C6	222-ILE	CD1	4.18
15	C8	222-ILE	CD1	3.72
16	C10	222-ILE	CD1	3.53
17	C12	222-ILE	CD1	3.85
18	01	222-ILE	CD1	4.13
19	C13	225-ALA	C8	3.64
20	04	225-ALA	. C8	4.02
21	04	228-ARG	CZ	3.96
22	C17	228-ARG	NH2	3.36
23	03	228-ARG	NH2	3.58
24	04	228-ARG	NH2	2.86
25	C10	256-MET	SD	3.70
26	C12	256-MET	SD	3.89
27	C10	256-MET	CE	3.88
28	C12	256-MET	CE	3.83
29	C11	259-MET	С	4.03
30	C11	259-MET	0	3.66
31	C15	259-MET	0	3.42
32	N1	259-MET	. 0	3.71
33	C1	259-MET	C8	4.20
34	C11	259-MET	C8	3.87
35	C13	259-MET	C8	4.09
36	C15	262-ARG	C8	4.03
37	C17	262-ARG	C8	3.58
38	03	262-ARG	C8	3.62
39	04	262-ARG	C8	3.85
40	C17	262-ARG	CD	4.10
41	04	262-ARG	CD	3.61
42	N1	263-ALA	N	3.71
43	C17	263-ALA	· CA	3.69
44	N1	263-ALA	СВ	3.46
45	03	266-ARG	NH1	3.93
46	N1	275-THR	0	3.62
47	N1	276-LEU	CA	3.51
48	N1 ·	276-LEU	С	3.92
49	C5	276-LEU	CD1	4.05
50	C19	276-LEU	CD1	4.04
51	C7	276-LEU	CD2	4.09
52	C9	276-LEU	CD2	3.95
53	C11	276-LEU	CD2	4.13
54	N1	276-LEU	CD2	4.17
55	C13	277-SER	N	4.14
56	C15	277-SER	N	3.79
	3.0	-// VEII	14	5.75

		history,		Tar spile fight
1	Dimit	mino Acid		
2 3 4	Atom	in full length a	Atom	Distance A
3	C17	277-SER	N	3.69
4	N1	277-SER	N	3.30
5	03	277-SER	N	3.19
6	C17	277-SER	CA	3.92
5 6 7 8 9	03	277-SER	CA	3.35
8	C13	277-SER	OG	3.92
9	C7 _	287-LEU	CD2	3.90
10	C18	290-GLY	С	4.04
11	C18	290-GLY	0	3.54
12	C18	291-GLY	CA	4.04
13	C18	292-LEU	N	4.20
14	C2	292-LEU	CG	4.18
15	C4	292-LEU	CG	3.86
16	C6	292-LEU	CG	4.01
17	C2	292-LEU	CD1	3.88
18	C4	292-LEU	CD1	4.02
19	02	292-LEU	CD1	4.07
20	C4	292-LEU	CD2	4.05
21	∥ C6	292-LEU	CD2	3.72
22	C8	292-LEU	CD2	3.69
23	C10	292-LEU	CD2	3.98
24	01	292-LEU	CD2	4.16
25	C20	299-ILE	CD1	3.87
26	C8	381-HIS	CD2	3.90 -
27	C10	381-HIS	CD2	3.84
28	01	381-HIS	GO2	3.40
29	01	381-HIS	CE1	3.72
30	C8	381-HIS	NE2	3.47
31	C10	381-HIS	NE2	3.51
32	01	381-HIS	NE2	2.64
33	C6	388-MET	CE	3.90
34	C8	401-PHE	CE1	4.19
35	01	401-PHE	CE1	3.37
36	C16	401-PHE	CZ	3.97
37	01	401-PHE	CZ	3.28
38	N1	502-H ₂ O	01	3.35
39	03	502-H ₂ O	01	2.56
40	03	503-H ₂ O	01	3.13
41	04	503-H ₂ O	01	3.72
42	04	504-H₂O	01	2.72

Legend to Table 8. The table lists the interactions with Dimit (DMT). The column headings are as follows:

^{#1} The atom of Dimit that interacts with the amino acid of the receptor. These are also numbered in figure 32.

^{49 #2} The amino acid in the full length rTRa that interacts with the ligand.

^{#3} The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

^{#4} The distance in A between Dimit and the protein atom.

2	Triac	Amino Acid	Amino Acid	
2 3 4 5 6 7 8 9	Atom	in full length a	Atom	Distance A
4	11	218-PHE	0	3.52
5	11	221-ILE	CD1	4.16
6	.∦ 11	221-ILE	CG1	3.92
7	∦ 11	222-ILE	CA	4.15
8		222-ILE	СВ	4.03
9	11	222-ILE	CG1	3.92
10	∥ C8	222-ILE	CD1	4.12
11	C10	222-iLE	CD1	3.77
12	C12	222-ILE	CD1	3.79
13	C13	225-ALA	СВ	4.17
14	C3	225-ALA	СВ	3.86
15	C10	256-MET	SD	3.45
16	C12	256-MET	SD	3.73
17	C10	256-MET	CE	3.66
18	C12	256-MET	CE	3.77
19 20	13	256-MET	CE	3.89
20 21	C1	259-MET	0	3.93
22	C11 03	259-MET	0	3.24
23	C1	259-MET	0	4.09
24	C13	259-MET 259-MET	СВ	3.89
25	C14	259-MET	0	3.74
26	C1	259-MET	СВ	3.96
27	C11	259-MET	СВ	3.89 3.68
28	C13	259-MET	СВ	4.01
29	C11	259-MET	CA	4.13
30	C13	259-MET	CA	4.20
31	13	260-SER	CA	4.10
32	∥ 13	260-SER	OG	4.19
33	C14	262-ARG	СВ	4.07
34	04	262-ARG	СВ	3.60
35	03	263-ALA	N	3.79
36	C14	263-ALA	N	4.12
37 38	03	263-ALA	CA	3.67
39	03	263-ALA	СВ	3.49
40	C11 C14	263-ALA	CB	4.00
41	03	266-ARG 266-ARG	CZ	3.89
42	03	266-ARG	CZ CZ	4.01
43	C14	266-ARG	NH1	3.03
44	03	266-ARG	NH1	3.25 3.00
45	04	266-ARG	NH1	2.82
46	C14	266-ARG	NH2	3.48
47	03	266-ARG	NH2	4.01
48	04	266-ARG	NH2	2.34
49	03	275-THR	C	4.02
50	C14	275-THR	Ö	4.20
51	03	275-THR	Ö	3.20
52	ОЗ ,	278-LEU	CA	3.11
53	03	276-LEU	С	3.52
54	03	276-LEU	N	4.04
55	C14	276-LEU	CA	3.98
56	03	276-LEU	CA	3.11

	Triac	mino Acid	Amino Acid	
	Atom	in full length a	Atom	Distance A
1	C14	276-LEU	С	3.98
2 3	03	276-LEU	СВ	3.95
. 3	02	276-LEU	CD1	4.03
4 5	11	276-LEU	CD1	4.10
2	C7	276-LEU	CD2	3.84
6	C9	276-LEU	CD2	3.73
7 8 9	CII -	276-LEU	CD2	4.06
8	02	276-LEU	CD2	4.10
	03	276-LEU	CD2	3.91
10	C13	277-SER	N .	4.06
11	C14	277-SER	N	3.13
12	04	277-SER	N	3.28
13	03	277-SER	N	3.05
14	C14	277-SER	CA	3.76
15	04	277-SER	CA	3.52
16	C3	277-SER	OG	3.87
17	C13	277-SER	OG	4.02
18	C14	277-SER	OG	4.14
19	12	290-GLY	0	3.57
20 21	12	292-LEU	CG	3.94
22	C4	292-LEU	CG	3.95
23	C6	292-LEU	CG	3.65
24	C8	292-LEU	CG	4.02
25	C2	292-LEU	CD1	4.11
26	C4	292-LEU	CD1	3.85
27	C6 I2	292-LEU	CD1	4.02
28	C4	292-LEU	CD2	3.98
29	C4 C6	292-LEU	CD2	4.11
30	C8	292-LEU	CD2	3.44
31	C10	292-LEU 292-LEU	CD2	3.28
32	01	292-LEU 292-LEU	CD2	3.88
33	13	292-LEO 299-ILE	CD2 CD1	3.35
34	C8	381-HIS	CD2	3.77
35	C10	381-HIS	CD2	3.87
36	01	381-HIS		3.90
37	01	381-HIS	GO2 CE1	3.20
38	C8	381-HIS	NE2	3.82 3.57
39	C10	381-HIS	NE2	3.5 <i>7</i> 3.52
40	01	381-HIS	NE2	3.52 2.64
41	01	388-MET	· CE	4.03
42	01	401-PHE	CE1	3.86
43	01	401-PHE	CZ	3.70
44	C13	460-H ₂ 0	01	4.00
45			<u> </u>	7.00
7.5				

44.44

Legend to Table 9. The table lists the interactions with Triac. The column headings are as follows: #1 The atom of Triac that interacts with the amino acid of the receptor. These are also numbered in figure 32.

^{#2} The amino acid in the full length rTRa that interacts with the ligand.

^{#3} The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

^{#4} The distance in A between Triac and the protein atom.

2	IpBR ₂ Atom	Amino Acid		·
_	IPBN ₂ Atom		Amino Acid	Distance
3	C16	in full length a	Atom	A
3 4 5 6 7	C16	215-PHE	CD1	4.01
5		215-PHE	CE1	3.78
5	BR1	218-PHE	0	3.24
7	BR1	218-PHE	С	3.98
. /	C16 _	218-PHE	СВ	3.81
8	C18	218-PHE	, CB	3.92
10	BR1	218-PHE	СВ	4.08
10	C18	218-PHE	CD2	3.92
11	C16	219-THR	CG2	3.45
12	BR1	221-ILE	CG1	3.81
13	BR1	221-ILE	CD1	4.07
14	BR1	222-ILE	СВ	3.81
15	BR1	222-ILE	CG1	3.97
16	C6	222-ILE	CD1	4.07
17	∥ C8	222-ILE	CD1	3.64
18	C10	222-ILE	CD1	3.50
19	C12	222-ILE	CD1	3.82
20	01	222-ILE	CD1	4.08
21	C13	225-ALA	СВ	3.76
22	04	225-ALA	СВ	4.01
23	04	228-ARG	CZ	3.92
24	C17	228-ARG	NH2	3.26
25	03	228-ARG	NH2	3.43
26	04	228-ARG	NH2	2.79
27	C10	256-MET	SD	3.65
28	C12	256-MET	SD	3.71
29	C10	256-MET	CE	3.90
30	C12	256-MET	CE	3.75
31	BR2	256-MET	CE	4.03
32	C11	259-MET	C	3.98
33	C11	259-MET	Ŏ	3.52
34	C15	259-MET	Ö	3.44
35	N1	259-MET	Ŏ	3.76
36	C11	259-MET	СВ	3.87
37	N1	262-ARG	C	4.03
38	C15	262-ARG	СВ	4.03
39	C17	262-ARG	СВ	3.56
40	03	262-ARG	СВ	3.55
41	04	262-ARG	- CB	3.91
42	C17	262-ARG	CD	4.09
43	04	262-ARG	CD	3.71
43 44 45	N1	263-ALA	N	3.61
45	N1	263-ALA	ĊA	3.59
46	N1	263-ALA	CB	3.54
47	03	266-ARG	NH1	3.93
48	N1	275-THR	Ö	3.43
49	N1	276-LEU	CA	3.46
50	N1	276-LEU	c	3.83
51	C5	276-LEU	CD1	4.02
52	C7	276-LEU	CD1	·
53	C9	276-LEU	CD2	4.00
54	C11	276-LEU	CD2 CD2	3.81 3.91
55	C13	270-LEO 277-SER	N CD2	12
I	0.10	2//-SER	IV IV	3.79

		(40/200)	ţ	SALANA
	IpBR₂ Atom	mino Acid	Amino Acid	Distance
	#	in full length a	Atom	A
1 2 3 4 5 6 7 8 9	C15	277-SER	N	3.63
2	∥ C17	277-SER	N	3.70
3	N1	277-SER	N	3.17
4	03	277-SER	N	3.37
5	C17	277-SER	CA	3.89
6	03	277-SER	CA	3.43
7	C13	277-SER	OG	3.66
8	02	287-LEU	CD1	4.05
19	C18	290-GLY	С	4.04
10	C18	290-GLY	0	3.48
11	C18	291-GLY	CA	4.02
12	C4	292-LEU	CG	3.89
13	C6	292-LEU	CG	4.02
14	C2	292-LEU	CD1	3.79
15	C4	292-LEU	CD1	3.96
16	02	292-LEU	CD1	3.97
17	C4	292-LEU	CD2	4.07
18	C6	292-LEU	CD2	3.75
19	C8	292-LEU	CD2	3.67
20	C10	292-LEU	CD2	3.92
21	BR2	299-ILE	CD1	3.68
22 23	C8	381-HIS	CD2	3.92
24	C10 01	381-HIS	CD2	3.78
2 4 25	01	381-HIS	GD2	3.50 -
26	C8	381-HIS	CE1	3.62
24 25 26 27	C10	381-HIS 381-HIS	NE2	3.36
28	01	381-HIS	NE2 NE2	3.34
29	C8	401-PHE	CE1	2.62
30	01	401-PHE	CE1	4.02
31	C16	401-PHE	CZ	3.19
32	01	401-PHE	CZ	4.03 3.06
33	03	502-H ₂ O	01	3.40
34	N1	502-H20	01	3.12
35	04	503-H ₂ O	01	3.20
36	C17	503-H20	01	3.04
37	03	503-H ₂ O	01	2.27
38	C15	504-H20	01	4.01
39	C17	504-H ₂ O	01	2.99
40	03	504-H2O	01	3.80
41	04	504-H₂O	. 01	1.78
امد			<u> </u>	

Legend to Table 10. The table lists the interactions with lpBr2. The column headings are as follows:

^{#1} The atom of lpBr2 that interacts with the amino acid of the receptor. These are also numbered in figure 32.

^{#2} The amino acid in the full length rTRa that interacts with the ligand.

^{#3} The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

^{#4} The distance in A between IpBr2 and the protein atom.

2	T3 Atom	Amino Acid	Amino Acid	
		in full length a	Atom	<u>Distance</u> A
3 4 5 6 7 8 9	12	215-PHE	CD1	4.08
4	11	218-PHE	0	3.19
5		218-PHE	СВ	3.99
6	∥ C4	218-PHE	СВ	4.04
7	11 •	218-PHE	С	3.79
8	11	218-PHE	СВ	3.99
19	11	221-ILE	CG1	4.01
10	11	222-ILE	СВ	3.95
11	11	222-ILE	CG1	3.91
12	C8	222-ILE	CD1	3.99
13 14	C10	222-ILE	CD1	3.57
15	C12	222-ILE	CD1	3.68
16	C13 C3	225-ALA	СВ	3.66
17	04	225-ALA 228-ARG	CB	4.04
18	04	228-ARG	NH1	3.23
19	C15	228-ARG	CZ NH2	3.45
20	03	228-ARG	NH2 NH2	3.54
21	04	228-ARG	NH2	3.90 2.86
22	C10	256-MET	SD	3.73
23	C12	256-MET	SD	3.90
24	C10	256-MET	CE	3.97
25	C12	256-MET	CE	3.92
26	13	256-MET	CE	3.89
27	C11	259-MET	C	3.95
28 29	C11	259-MET	0 0	3.59
30	C14 N1	259-MET		3.51
31	C1	259-MET 259-MET	0	3.88
32	C11	259-MET	CB CB	4.06
33	C13	259-MET	СВ	3.77 3.96
34	C15	262-ARG	СВ	3.61
35	C14	262-ARG	СВ	4.02
36	03	262-ARG	СВ	3.65
37	04	262-ARG	СВ	3.92
38	04	262-ARG	CD	3.72
39	N1	263-ALA	N	3.81
40 41	N1	263-ALA	CA	3.81
42	N1 N1	263-ALA 275-THR	. CB	3.63
43	N1	275-17R 276-LEU	0	3.54
44	N1	276-LEU 276-LEU	CA C	3.38 3.73
45	C5	276-LEU	CD1	4.00
46	· C7	276-LEU	CD1	4.05
47	02	276-LEU	CD1	4.03
48	C7	276-LEU	CD2	3.80
49	C9	276-LEU	CD2	3.70
50	C11	276-LEU	CD2	4.01
51	C14	277-SER	N	3.67
52	C15	277-SER	N	3.62
53 54	N1	277-SER	N	3.07
54 55	03 C15	277-SER	N	3.24
-J [C15	277-SER	CA	3.77

	T3 Atom	mino Acid	Amino Acid	
		in full length a	Atom	<u>Distance</u>
1	03	277-SER		Α
1 2 3 4 5 6 7 8 9	C13	277-SER	CA	3.34
2	12		OG	3.92
1	li .	290-GLY	0	3.50
4	C4	292-LEU	CG	3.95
2	C8	292-LEU	CG	3.83
0	C2	292-LEU	CD1	4.07
7	C4	292-LEU	CD1	3.99
8 -	C4	292-LEU	CD2	4.09
9	C6	292-LEU	CD2	3.58
10		292-LEU	CD2	3.50
11	∥ C10	292-LEU	CD2	3.96
12	01	292-LEU	CD2	3.71
13	13	299-ILE	CD1	3.74
14	C8 .	381-HIS	CD2	3.94
15	C10	381-HIS	CD2	3.97
16	01	381-HIS	CD2	3.39
17	01	381-HIS	CD1	3.82
18	C8	381-HIS	NE2	3.47
19	C10	381-HIS	NE2	3.55
20	01	381-HIS	NE2	2.70
21	01	388-MET	CE	3.88
22	01	401-PHE	CE1	3.52
23	01	401-PHE	CZ	3.32
24	C14	502-H20	01	4.01
25	C15	502-H2O	01	3.61
26	03	502-H20	01	2.51
27	C15	503-H2O	01	3.31
28	04	503-H ₂ O	01	3.10
29	N1	502-H ₂ O	01	3.10
30	03	503-H2O	01	2.81
31	C15	504-H2O	01	
32	04	504-H2O	01	3.92
		304-H2O		2.73
33				

Legend to Table 11. The table lists the interactions with T3. The column headings are as follows:

34 35

36 37 38

39 40

41

^{#1} The atom of T3 that interacts with the amino acid of the receptor. These are also numbered in figure 32.

^{#2} The amino acid in the full length rTRa that interacts with the ligand.

^{#3} The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

^{#4} The distance in A between T3 and the protein atom.

2	Triac	Amino Acid	Amino Acid	
3	Atom	in full length hTR β	Atom	Distance A
2 3 4 5	12	269-PHE	CD1	3.75
. 3	12	269-PHE	CE1	3.88
6	l1	272-PHE	C	4.03
7 8	11	272-PHE	0	3.54
9	11 -	275-ILE	CG1	3.93
10	11	276-ILE	CG1	4.02
11	C3	279-ALA	CB	3.81
12	C13 C10	279-ALA	CB	3.87
13	C10 C12	310-MET	SD	3.72
14	C12 C10	310-MET 310-MET	SD CE	3.78
15	C12	310-MET	CE	4.02
16	13	310-MET	CE	3.92
17	C13	313-MET	CA	3.93
18	C11	313-MET	C	3.94 3.72
19	C1	313-MET	0	3.79
20	C11	313-MET	Ö	3.79
21	C13	313-MET	Ö	3.55
22	C1	313-MET	СВ	4.00
23	C11 ,	313-MET	СВ	3.82
24	C13	313-MET	СВ	3.76
25	C13	313-MET	CG	3.88
26	03	316-ARG	CB	3.99
2/	04	317-ALA	CA	4.08
21 22 23 24 25 26 27 28 29	04	317-ALA	CA	4.10
30	C11	317-ALA 317-ALA	CB	3.70
31	04	317-ALA 317-ALA	CB CB	4.10
32	04	320-ARG	NH1	4.06 3.58
33	03	320-ARG	NH2	3.55
34	04	320-ARG	NH2	4.04
35	04	329-THR	0	3.55
36	04	330-LEU	CA	3.42
37	04	330-LEU	C	3.77
38	C3	330-LEU	СВ	4.06
39	C5	330-LEU	СВ	4.08
40 41	C1 C3	330-LEU	CD2	4.07
42	C5	330-LEU 330-LEU	CD2 CD2	4.00
43	C7	330-LEU	CD2	3.73 3.51
44	C9	330-LEU	CD2	3.54
45	C11	330-LEU	CD2	3.86
46	C15	331-ASN	N	3.55
47	03	331-ASN	N	3.74
48	04	331-ASN	N N	3.12
49	03	331-ASN	CA	4.02
50	12	344-GLY	0	3.87
51	C6	346-LEU	CD2	3.87
52	C8	346-LEU	CD2	3.84
53 54	01	346-LEU	CD2	3.91
55	13 C8	353-ILE	CD1 CD2	3.51
56	C8 C10	435-HIS 435-HIS	CD2 CD2	3.93
	0.0	-1 30-HI3	CDZ	3.79

	1
	2
	3
	4
	5
	6
	7
	8
	9
1	0

Triac	mino Acid	Amino Acid	
Atom	in full length hTR β	Atom	Distance A
01	435-HIS	CD2	3.33
01	435-HIS	CE1	3.81
C8	435-HIS	NE2	3.42
C10	435-HIS	NE2	3.33
01	435-HIS	NE2	2.67
01	442-MET	SD	3.96
01 -	442-MET	CE	3.72
12	442-MET	SD	4.01
01	455-PHE	CE1	3.92
01	455-PHE	CZ	3.50

14

18

19

20

21

Legend to Table 12. The table lists the interactions with Triac. The column headings are as

- 15 The atom of Triac that interacts with the amino acid of the receptor. These are also #1 16 numbered in figure 32. 17
 - The amino acid in the full length hTR\$ that interacts with the ligand.
 - #3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
 - #4 The distance in A between Triac and the protein atom.

2	GC1	Amino Acid	1 Amina Asid	
2 3 4 5 6 7 8 9	Atom	in full length TR &	Amino Acid Atom	District
4	C16	269-PHE	CE1	Distance A
5	C19	272-PHE	O	3.99
6	C16	272-PHE	СВ	3.85
. 7	C16	273-THR	CG2	3.98
8	C19 -	275-ILE	CG1	3.76
9	C19	276-ILE	CA CA	3.98 3.98
10	C2	276-ILE	CD1	3.88
11	C8	276-ILE	CD1	3.77
12	C10	276-ILE	CD1	3.58
13	C12	276-ILE	CD1	3.62
14	C19	276-ILE	CD1	3.56
15	C1	279-ALA	СВ	3.68
16	СЗ	279-ALA	СВ	3.56
17	O5	279-ALA	СВ	3.11
18	04	279-ALA	СВ	3.90
19	03	282-ARG	cz	3.53
20	C17	282-ARG	NH1	3.87
21	03	282-ARG	NH1	3.20
22	04	282-ARG	NH1	3.85
23	C17	282-ARG	NH2	3.63
24	03	282-ARG	NH2	3.00
25	C10	310-MET	SD	3.86
26	C12	310-MET	SD	3.91
27	C11	313-MET	С	3.85
28	C11	313-MET	0	3.41
29	C15	313-MET	0	3.87
30	C20	313-MET) 0	3.99
31	C11	313-MET	СВ	3.79
32	C1	313-MET	CG	3.94
33	C11	313-MET	CG	3.91
34 35	05	313-MET	CG	3.87
36	04	313-MET	CG	3.79
37	C20 C17	314-SER	CA	4.00
38	C17	316-ARG 316-ARG	СВ	3.95
39	03	316-ARG	CD CD	3.80
40	04	316-ARG	CD	3.83
41	C20	317-ALA	CB	3.51 3.93
42	C7	330-LEU	CD2	3.56
43	C9	330-LEU	CD2	3.63
44	C21	330-LEU	CD2	3.90
45	05	331-ASN	N	3.62
46	C15	331-ASN	N	3.67
47	C18	344-GLY	ö	3.60
48	C18	346-LEU	CG	3.89
49	C6	346-LEU	CD2	3.77
50	C8	346-LEU	CD2	3.80
51	C10	435-HIS	CD2	3.89
52	01	435-HIS	CD2	3.64
53	01	435-HIS	CE1	3.79
54	C8	435-HIS	NE2	3.44
4			 	

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2
3
4
5

GC1 Atom	in full length TR β	Amino Acid Atom	Distance A
C10	435-HIS	NE2	3.33
O1	435-HIS	NE2	2.77
O1	455-PHE	CE1	3.40
O1	455-PHE	CZ	3.22

Legend to Table 13. The table lists the interactions with GC1. The column headings are as follows:

#1 The atom of GC1 that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length hTR\$ that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between GC1 and the protein atom.

Table 14
Coordination Structure of TR-σ and Dimit

Coordination	R ₁	R ₂	R ₃	R ₅	R ₆	R'2	R' ₃	R'	R'5	R'6	
Structure	<u> </u>	<u> </u>			<u> </u>					"	
	-CH ₂ - CH(NH ₂)(CO ₂)H	-H	-CH₃	-CH₃	-Н	-Н	-CH(CH₃	₂ -Ol	1 -Н	-H	(
AA							215	T	7	7	T-
SS							Н3			+	+
AA			218				218		_	1	╁
SS .	-		НЗ		1		НЗ	+-	 	+	┿
AA							219		_	+	+
SS						1	НЗ		 	+	+
AA			221	Î	1	1			1	+	+
SS			НЗ				<u> </u>	_	+	 	+
AA							222	222	222	222	+
SS							НЗ	H3	НЗ	НЗ	+-
AA	225					T		+-	† –	 	+-
SS	Н3							†	 	 	+
AA '	228								1	 	+
SS	Н3							<u>† </u>		 	†
AA				-					256	256	
SS									H5-	H5-	
AA	259	-			259			┼	H6	Н6	—
SS	H5-H6				H5-H6	-		├		 	1
AA	262					-		 	-		┼
s	H5-H6	-				 		├—			┼—
AA	263	_						+	 		┼
s	H5-H6							+	 		-
NA	266							╁──	-	-	├
S	loop										┼
\A	275		$\neg \uparrow$		• • • • • • • • • • • • • • • • • • • •			 	 		
s	S3							 	 		
VA	276		276	276	276		·		 		
S	S 3		S3	S3	S 3						
A	277										
S	loop										
A							290-291				
S							loop				
A					•	292	292	292	292		29
S						loop	loop	loop	loop		loo
A				299							
S				Н8							
Α								381	381		
S								H11	H11		
Α							388				
S							H11				
A							401	401			
s							H12	H12			
A F	10H502/H0H5 03/H0H504										
5			 -								

AA = Amino Acid

Table 15 Coordination Structure of TR-α and Triac

Coordination	R ₁	To		ТВ	T 6	T D/	I D/	57	T 54		
Coordination	D1	R ₂	R ₃	R ₅	R ₆	R′2	R'3	R′₄	R's	R' ₆	X
Structure	-			•	ł						
	-CH₂-COOH	-H	-1	-1	-Н	-H	-1	-ОН	-H	'-H	0
AA			218							T	T
SS	•		НЗ								
AA			221								
SS			НЗ			1					
AA							222	222	222	222	
SS						1	нз	НЗ	НЗ	нз	
AA	225						1				
SS	Н3										
AA .				256					256	256	
SS				H5-H6			1		H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5- H6						
AA	262				1110	-		ļ	ļ		
SS	H5-H6						 				
ĀĀ	263					-		 			
SS	H5-H6	\dashv				╁	-	-			
AA	266					 - -	 -				
SS	loop	-				 	 		-		
AA	275					 	 				
SS	53	一十					 				
AA	276	\dashv	276	276	276		-				
ss	S3	-	S3	<u>\$3</u>	<u>S3</u>		 				
AA	277	十					 				
ss	loop									 	
AA		-					290				
ss		\neg		-	<u> </u>	\vdash	loop				· · ·
AA		_				292	292	292	292		292
SS		_				loop	loop	loop	loop		loop
AA		_		299							
SS		十		Н8		•					
AA								381	381		
SS		_						H11	H11		
AA		一						388			
SS		$\neg \vdash$						H11			
AA		\neg					401	401	-		
SS		$\neg \vdash$					H12	H12			

AA = Amino Acid

Table 16
Coordination Structure of TR-α and IpBr2

Coordination						· · · · · · · · · · · · · · · · · · ·	-α and I	<u> </u>			,
Structure	R ₁	R ₂	R ₃	R₅	R ₆	R′2	1	R' ₄	R's	R'6	X
	-CH2-CH(NH2)(CO2)H	-H	-Br	-Br	-H	-H	-CH(CH ₃)	OH	-H	-H	-
AA				Ţ			215	1	T	T	Ť
SS				1	1		Н3			 	+
AA			218			T	218			 	+
SS			H3			1	НЗ			 	+
AA							219			<u> </u>	
SS						1	НЗ		<u> </u>		+
AA			221					1	· ·		+
SS			НЗ			1 .					
AA						1	222	222	222	222	+
SS							НЗ	НЗ	НЗ	нз	
AĀ	225				<u> </u>			_			1
SS	Н3								 		+
AA	228					† ·		+	1		+
SS	Н3										†
AA					256			1	256	256	1
SS					H5-H6				H5-H6	H5-	
						1		Ì		Н6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop									·	
AA	275										
SS	\$3										
AA	276		276	276	276						
SS	\$3		S3	S3	S3						
AA	277										
SS											
AA		ļ	1		•		290-	1 1	- 1		
00						•	291				
SS						200	loop	000	000		
AA SS		 -				292	292	292	292		292
				303		loop	loop	loop	loop		loop
AA SS	<u>-</u>			299						·	
		-		Н8				004			
AA								381	381		
SS		_					404	H11	H11		
AA							401	401			
SS	11011505						H12	H12			
NA	HOH5O2/HOH 5O3/HOH5O4								ı		
SS			$\neg \uparrow$		·						

AA = Amino Acid

Table 17
Coordination Structure of TR-a and Dimit

Coordination	R,	R ₂	R ₃	R ₅	R ₆	R'2	R'	3 R'4	R'5	R'6	ΙX
Structure			1	<u>L.</u> .	İ				*		``
	-CH ₂ - CH(NH ₂)(CO ₂)H	-H	-1	-1	-H	-H	-1	-OH	-H	-н	0
AA			T				21	5	T	1	T
SS							НЗ				_
AA			218			218	3	1		 	+-
SS	•		НЗ			H3					+
AA			221			1			1	 -	+-
SS			НЗ		1				†	+	_
AA							222	2 222	222	222	+
SS							НЗ	НЗ	НЗ	НЗ	┼─
AA	225					1	 	1	 		<u> </u>
SS	НЗ				† · · · · ·		 	1		 	
AA	228				1			\top	 	 	
SS	нз				İ		 	1	 	†	
AA					256			1	256	256	 -
SS				i	H5-	1		+	H5-	H5-H6	
					Н6			1	Н6		
AA	259				259						
SS	H5-H6				H5- H6						
AA	262			-		 	 	 			
ss	H5-H6						 	 	<u> </u>	 	
AA	263						 	 		 	
SS	H5-H6					 	 	;			
AA	275						 	 			
ss	S 3				<u> </u>		-				
AA	276		276	276	276		 				
ss	S 3		S3	S 3	S 3		<u> </u>	 			
AA	277				-						•
ss											
AA						 	290				
SS							loop	 			
AA						292	292	292	292		292
ss						loop	loop		loop		loop
AA A				299				1			юор
SS				Н8				 			
NA								381	381		
ss		-+						H11	H11		
NA			-+					388			
s			+					H11			
NA I			-+				401	401			
S				·				H12			
	НОН502/НОН		+				2	,,,,,			
J	503/H0H504				ſ				ľ	İ	
s		一十	一十					- 		 	

AA = Amino Acid SS = Secondary Structure

Table 18
Coordination Structure of TR-β and Triac

Coordination Structure	R1	R2	R3	R5	R6	R2'	R3	R4	R5	R6	7
	-CH ₂ CO ₂ H	Н		1	Н	Н		ОН	Т н		۲-
AA							269	7	T		T
SS	-						НЗ			 	十一
AA			272							 	╁╴
SS			НЗ							 	1
AA			275							 	
SS			H3					-		 	
AA			276							†	
SS			НЗ								
AA	279	279		Ì						<u> </u>	
SS	НЗ	Н3									
AA				310					310	310	
SS				H5- H6				1	H5- H6	H5-H6	
AA	313				313			+			
SS	H5-H6				H5- H6		,				
AA	316							+	-		
SS	H5-H6							+	 		
AA	317				317		317	 			
SS	Н5-Н6				H5- H6		H5- H6				
AA	320							 			-
SS	H5-H6							 			
AA	329							1-			
SS	S3						·				
AA	330	330	330	330	330						
SS	S3	S3	S3	S3	S3						
AA	331						-				
SS	loop										
AA							344				
SS							loop		-		
AA							346	346			
SS							loop	loop			
AA .				353							
SS				Н8							
AA								435	435		
SS								H11	H11		
AA .							442	442			
SS							H11.	H11			
NA .								455			
SS								H12			

AA = Amino Acid

Table 19
Coordination Structure of TR-β and GC1

Coordination Structure	R₁	R ₂	R ₃	R ₅	R ₆	R2	R3	R4	R5	R6	Τx
Structure	-O-CH₂CO₂H	' н	CH ₃	CH ₃	. Н	H	L CH(CH₃) OH	Н Н	<u> </u>	CH
				3			_		• • •	П	2
AA		<u> </u>				<u></u>	269				Τ
SS					<u> </u>	<u> </u>	Н3				
AA			272								
SS			НЗ		<u> </u>						
AA		<u> </u>	273				273				
SS	·		НЗ				НЗ				
AA			275								
SS	<u> </u>		НЗ								
AA			276					276	276	276	
SS			Н3					НЗ	Н3	НЗ	
AA	279	279									
SS	нз	НЗ									
AA	282										\vdash
SS	НЗ										
AA				310					310	310	
SS				H5-H6					H5- H6	Н5-Н6	
AA	313				313			 			
ss	Н5-Н6				H5- H6						
AA							314	<u> </u>			
ss							H5-H6				
AA	316					- 		 			
ss	H5-H6										-
AA	·						317				
ss						-	H5-H6				
AA	320					_					
ss	H5-H6										
AA	329					一甘					
SS	S3					$\neg +$					
AA	330			330		-					
SS	S3			S3		, 					
AA	331					$\neg \dagger$		-			
SS	loop					_	-				-
NA						-	344				
SS					-	\dashv	loop				
NA.							346	346			
S						_	loop	loop			\dashv
VA				353		\dashv					
S		\dashv		Н8		-+		╌╌┤			
IA		_	-+	+		\dashv		435	435		
						\dashv		H11	H11		
			-+					455			
s						-	1	H12			

AA = Amino Acid

APPENDIX 3

TR DMT.PDB

REMARK TR dmit full length numbering REMARK REMARK Rfactor 0.205 Rfree 0.227 REMARK Resolution 15. 2.2 all reflections **REMARK** REMARK Three cacodylate-modified cysteines (CYA) REMARK Cya334, Cya380, Cya392 REMARK cacodylate modeled as single arsenic atom REMARK REMARK side chain of certain residues modeled as ALA due to poor density; REMARK however, residue name reflects true residue for clarity REMARK REMARK clone obtained from Murray et. al. REMARK deposited sequence confirmed, REMARK differing from that reported by Thompson et. al. REMARK in the following codons: REMARK 281 Thr - Ala REMARK 285 Lys - Glu REMARK identical to that reported by Mitsuhashi et. al. REMARK gb:RNTRAVI X07409 JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY, M.J.MACDONALD JRNL **AUTH 2 H.C.TOWLE** JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES FOR TWO JRNI. TITL 2 DISTINCT THYROID HORMONE RECPTORS JRNL REF **JBC** V. 263 25 1988 AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS JRNL JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR **EXPRESSED** JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM JRNL REF SCIENCE V. 237 1987 JRNL . AUTH T.MITSUHASHI, G.TENNYSON, V.NIKODEM NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY **JRNL** TITL **ALTERNATIVE** TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE **JRNL** TRANSCRIPT JRNL NUC. ACIDS. RES. REF V. 16 12 1988 ATOM 1 N ARG 157 68.504 8.445 5.651 1.00 68.93 ATOM 2 CA ARG 157 67.886 9.543 6.398 1.00 56.98 ATOM 3 CB ARG 157 68.769 10.789 6.324 1.00 59.25

70.147 10.632 6.932 1.00 58.90

ATOM

4 CG ARG 157

ATOM	· 5 CD ARG 157	70.068 10.422 8.425 1.00 59.37
ATOM	6 NE ARG 157	71.392 10.446 9.036 1.00 63.94
ATOM	7 CZ ARG 157	71.613 10.329 10.341 1.00 64.39
ATOM	8 NH1 ARG 157	70.596 10.182 11.179 1.00 62.14
ATOM	9 NH2 ARG 157	72.855 10.365 10.808 1.00 65.56
ATOM	10 C ARG 157	66.500 9.881 5.854 1.00 48.97
ATOM	11 O ARG 157	66.351 10.203 4.674 1.00 48.61
ATOM	12 N PRO 158	65.469 9.818 6.712 1.00 41.90
ATOM	13 CD PRO 158	65.550 9.366 8.112 1.00 41.06
ATOM	14 CA PRO 158	64.083 10.114 6.333 1.00 39.34
ATOM	15 CB PRO 158	63.286 9.704 7.576 1.00 37.89
ATOM	16 CG PRO 158	64.260 9.883 8.693 1.00 42.40
ATOM	17 C PRO 158	63.814 11.573 5.930 1.00 37.10
ATOM	18 O PRO 158	64.189 12.517 6.636 1.00 33.31
ATOM	19 N GLU 159	63.171 11.733 4.778 1.00 30.56
ATOM	20 CA GLU 159	62.821 13.038 4.231 1.00 24.26
ATOM	21 CB GLU 159	62.553 12.904 2.727 1.00 19.19
ATOM	22 CG GLU 159	63.788 12.677 1.874 1.00 20.60
ATOM	23 CD GLU 159	64.407 13.971 1.390 1.00 26.54
ATOM	24 OE1 GLU 159	63.649 14.929 1.115 1.00 30.85
ATOM	25 OE2 GLU 159	65.649 14.027 1.268 1.00 28.35
ATOM	26 C GLU 159	61.549 13.520 4.909 1.00 23.26
ATOM	27 O GLU 159	60.906 12.765 5.643 1.00 26.86
ATOM	28 N PRO 160	61.200 14.806 4.729 1.00 22.72
ATOM	29 CD PRO 160	61.981 15.916 4.153 1.00 17.87
ATOM	30 CA PRO 160	59.969 15.292 5.359 1.00 19.90
ATOM	31 CB PRO 160	60.004 16.799 5.070 1.00 14.42
ATOM ATOM	32 CG PRO 160 33 C PRO 160	61.465 17.109 4.919 1.00 12.87
ATOM	33 C PRO 160 34 O PRO 160	58.747 14.623 4.701 1.00 23.68 58.730 14.383 3.491 1.00 24.72
ATOM	35 N THR 161	58.730 14.383 3.491 1.00 24.72 57.749 14.281 5.506 1.00 22.19
ATOM	36 CA THR 161	56.542 13.660 4.985 1.00 19.50
ATOM	37 CB THR 161	55.691 13.031 6.125 1.00 21.50
ATOM	38 OG1 THR 161	55.163 14.062 6.972 1.00 20.33
ATOM	39 CG2 THR 161	56.537 12.078 6.959 1.00 19.48
ATOM	40 C THR 161	55.744 14.765 4.298 1.00 22.86
ATOM	41 O THR 161	56.040 15.949 4.481 1.00 27.68
ATOM	42 N PRO 162	54.720 14.403 3.504 1.00 20.36
ATOM	43 CD PRO 162	54.280 13.050 3.113 1.00 16.55
ATOM	44 CA PRO 162	53.924 15.435 2.830 1.00 21.97
ATOM	45 CB PRO 162	52.780 14.633 2.210 1.00 18.17
ATOM	46 CG PRO 162	53.422 13.316 1.905 1.00 18.01
ATOM	47 C PRO 162	53.399 16.467 3.826 1.00 22.56
ATOM	48 O PRO 162	53.461 17.675 3.567 1.00 21.73
ATOM	49 N GLU 163	52.912 15.976 4.967 1.00 25.28
ATOM	50 CA GLU 163	52.357 16.816 6.030 1.00 26.64
ATOM	51 CB GLU 163	51.743 15.962 7.144 1.00 30.22

ATOM	52 CG GLU 163	50.514 15.131 6.748 1.00 44.99
ATOM	53 CD GLU 163	50.836 13.950 5.831 1.00 48.88
ATOM	54 OE1 GLU 163	
ATOM	55 OE2 GLU 163	51.895 13.309 6.015 1.00 44.23
ATOM	56 C GLU 163	53.414 17.731 6.634 1.00 27.65
ATOM	57 O · GLU 163	53.114 18.862 7.034 1.00 29.30
ATOM	58 N GLU 164	
ATOM	59 CA GLU 164	11 11 11 11 11 11 11 11 11 11 11 11 11
ATOM		
ATOM		56.901 17.109 7.657 1.00 14.78
		56.552 16.196 8.825 1.00 21.11
ATOM	62 CD GLU 164	57.669 15.249 9.198 1.00 20.35
ATOM	63 OE1 GLU 164	58.605 15.071 8.392 1.00 28.55
ATOM	64 OE2 GLU 164	57.610 14.677 10.302 1.00 28.25
ATOM	65 C GLU 164	56.200 19.097 6.306 1.00 24.62
ATOM	66 O GLU 164	56.574 20.183 6.741 1.00 32.05
ATOM	67 N TRP 165	56.174 18.817 5.003 1.00 28.22
ATOM	68 CA TRP 165	56.576 19.825 4.021 1.00 22.99
ATOM	69 CB TRP 165	56.575 19.262 2.605 1.00 17.37
ATOM	70 CG TRP 165	57.876 18.633 2.210 1.00 10.74
ATOM	71 CD2 TRP 165	59.153 19.283 2.109 1.00 11.74
ATOM	72 CE2 TRP 165	60.075 18.319 1.648 1.00 9.97
ATOM	73 CE3 TRP 165	59.606 20.583 2.365 1.00 13.88
ATOM	74 CD1 TRP 165	58.074 17.343 1.832 1.00 9.17
ATOM	75 NE1 TRP 165	59.390 17.145 1.486 1.00 16.55
ATOM	76 CZ2 TRP 165	61.427 18.613 1.436 1.00 13.37
ATOM	77 CZ3 TRP 165	60.954 20.874 2.156 1.00 16.15
ATOM	78 CH2 TRP 165	61.846 19.892 1.696 1.00 17.42
ATOM	79 C TRP 165	55.634 21.015 4.115 1.00 21.44
ATOM	80 O TRP 165	56.041 22.149 3.865 1.00 22.12
ATOM	81 N ASP 166	54.373 20.747 4.456 1.00 21.29
ATOM	82 CA ASP 166	53.369 21.796 4.621 1.00 25.77
ATOM	83 CB ASP 166	51.972 21.196 4.808 1.00 26.02
ATOM	84 CG ASP 166	51.428 20.559 3.539 1.00 33.01
ATOM	85 OD1 ASP 166	51.874 20.932 2.434 1.00 29.48
ATOM	86 OD2 ASP 166	50.537 19.692 3.649 1.00 34.47
ATOM	87 C ASP 166	53.732 22.637 5.842 1.00 27.91
ATOM	88 O ASP 166	53.744 23.865 5.767 1.00 31.28
ATOM	89 N LEU 167	54.046 21.966 6.951 1.00 25.57
ATOM	90 CA LEU 167	54.439 22.640 8.187 1.00 28.28
ATOM		
ATOM		
ATOM		53.945 21.347 10.455 1.00 41.75
	•	54.765 20.640 11.532 1.00 39.15
ATOM		53.374 22.647 11.008 1.00 39.20
ATOM	95 C LEU 167	55.636 23.532 7.902 1.00 22.19
ATOM	96 O LEU 167	55.671 24.700 8.302 1.00 29.51
ATOM	97 N ILE 168	56.610 22.957 7.206 1.00 15.01
ATOM	98 CA ILE 168	57.846 23.632 6.833 1.00 18.03

ATOM .. 99 CB ILE 168 58.756 22.668 6.040 1.00 11.37 **ATOM** 100 CG2 ILE 168 59.890 23.413 5.367 1.00 16.36 **ATOM** 101 CG1 ILE 168 59.289 21.580 6.975 1.00 21.63 **ATOM** 102 CD1 ILE 168 60.095 20.501 6.287 1.00 21.03 **ATOM** 103 C ILE 168 57.579 24.897 6.022 1.00 22.54 **ATOM** 104 O- ILE 168 58.155 25.948 6.300 1.00 24.88 **ATOM** 105 N HIS 169 56.682 24.800 5.045 1.00 25.70 106 CA HIS **ATOM** 169 56.337 25.934 4.190 1.00 21.28 **ATOM** 107 CB HIS 169 55.411 25.493 3.057 1.00 22.29 **ATOM** 108 CG HIS 169 56.047 24.543 2.091 1.00 23.11 109 CD2 HIS **ATOM** 169 57.348 24.265 1.839 1.00 16.86 **ATOM** 110 ND1 HIS 169 55.312 23.721 1.263 1.00 25.30 **ATOM** 111 CE1 HIS 169 56.130 22.974 0.546 1.00 15.89 112 NE2 HIS ATOM 169 57.371 23.283 0.878 1.00 25.38 **ATOM** 113 C HIS 169 55.664 27.048 4.976 1.00 18.32 **ATOM** HIS 114 O 169 56.033 28.215 4.842 1.00 21.53 VAL **ATOM** 115 N 170 54.679 26.685 5.795 1.00 17.13 **ATOM** 116 CA VAL 170 53.957 27.661 6.607 1.00 21.29 117 CB VAL **ATOM** 170 52.808 26.991 7.399 1.00 24.33 **ATOM** 118 CG1 VAL 170 52.164 27.985 8.354 1.00 23.78 ATOM 119 CG2 VAL 170 51.760 26.439 6.435 1.00 18.87 **ATOM** 120 C VAL 170 54.910 28.382 7.567 1.00 24.69 **ATOM** 121 O VAL 170 7.637 1.00 28.77 54.912 29.616 **ATOM** 122 N ALA 171 55.759 27.609 8.245 1.00 20,35 **ATOM** 123 CA ALA 56.722 28.148 171 9.202 1.00 19.61 **ATOM** 124 CB ALA 171 57.393 27.013 9.977 1.00 17.52 **ATOM** 125 C ALA 171 57.775 29.026 8.531 1.00 20.91 **ATOM** 126 O **ALA** 171 58.102 30.105 9.041 1.00 21.98 **ATOM** 58.308 28.571 127 N THR 172 7.398 1.00 18.94 **ATOM 128 CA THR** 172 59.313 29.342 6.668 1.00 19.55 **ATOM** 129 CB THR 59.820 28.594 172 5.413 1.00 20.49 **ATOM** 130 OG1 THR 172 60.394 27.336 5.795 1.00 20.66 **ATOM** 131 CG2 THR 172 60.894 29.418 4.702 1.00 20.44 **ATOM** 132 C THR 6.254 1.00 23.26 172 58.730 30.697 **ATOM** 133 O THR 172 59.403 31.724 6:334 1.00 24.32 **ATOM** 134 N GLU 173 57.468 30.694 5.836 1.00 27.42 135 CA GLU **ATOM** 173 56.797 31.922 5.434 1.00 27.68 **ATOM** 136 CB GLU 173 55.477 31.605 4.728 1.00 24.51 **ATOM** 137 CG GLU 173 54.652 32.836 4.338 1.00 39.69 **ATOM** 138 CD GLU 173 55.396 33.814 3.426 1.00 47.72 **ATOM** 139 OE1 GLU 173 55.019 35.009 3.417 1.00 48.26 **ATOM** 140 OE2 GLU 173 56.344 33.398 2.717 1.00 49.61 **ATOM** 141 C GLU 173 56.557 32.834 6.641 1.00 25.68 **ATOM** 142 O **GLU** 173 56.773 34.046 6.559 1.00 23.39 **ALA ATOM** 143 N 174 56.119 32.245 7.755 1.00 25.19 **ATOM** 144 CA ALA 174 55.863 32.989 8.993 1.00 22.25 **ATOM** 145 CB ALA 174 55.450 32.030 10.111 1.00 15.95

ATOM -146 C ALA 174 57.125 33.747 9.391 1.00 23.22 **ATOM** 147 O **ALA** 174 57.076 34.918 9.768 1.00 24.52 **ATOM** 148 N HIS 175 58.261 33.073 9.275 1.00 20.97 **ATOM** 149 CA HIS 175 59.544 33.665 9.606 1.00 19.55 **ATOM** 150 CB HIS 175 60.625 32.577 9.649 1.00 16.19 **ATOM** 151 CG HIS 175 62.016 33.104 9.835 1.00 18.89 **ATOM** 152 CD2 HIS 175 63.148 32.901 9.119 1.00 16.05 **ATOM** 153 ND1 HIS 175 62.359 33.962 10.859 1.00 13.83 ATOM 154 CE1 HIS . 175 63.642 34.265 10.765 1.00 15.87 **ATOM** 155 NE2 HIS 175 64.143 33.635 9.718 1.00 19.19 **ATOM** 156 C HIS 175 59.934 34.757 8.617 1.00 21.28 **ATOM** 175 157 O HIS 60.274 35.869 9.014 1.00 25.12 **ATOM** 158 N ARG 176 59.891 34.436 7.329 1.00 26.73 **ATOM 159 CA ARG** 176 60.266 35.387 6.292 1.00 27.13 **ATOM** 160 CB ARG 176 60.156 34.748 4.914 1.00 36.00 **ATOM** 161 CG ARG 176 61.286 33.795 4.602 1.00 43.20 **ATOM** 162 CD ARG 176 61.197 33.334 3.170 1.00 50.07 **ATOM** 163 NE ARG 176 62.316 32.477 2.813 1.00 58.20 **ATOM** 164 CZ ARG 176 62.266 31.548 1.867 1.00 67.22 **ATOM** 165 NH1 ARG 176 61.143 31.358 1.182 1.00 67.62 **ATOM** 166 NH2 ARG 176 63.336 30.806 1.612 1.00 70.56 **ATOM** 167 C **ARG** 176 59.487 36.688 6.325 1.00 23.97 **ATOM** 168 O **ARG** 176 6.209 1.00 24.52 60.073 37.760 **ATOM** 169 N **SER** 177 58.177 36.598 6.515 1.00 23.60 **ATOM** 170 CA SER 177 57.341 37.789 6.565 1.00 26.36 **ATOM** 171 CB SER 177 55.865 37.407 6.439 1.00 21.93 **ATOM** 172 OG SER 177 55.495 36.459 7.423 1.00 25.97 -ATOM 173 C SER 177 57.557 38.623 7.829 1.00 28.76 174 O **ATOM SER** 177 57.084 39.761 7.907 1.00 33.09 **ATOM** 175 N THR 178 58.257 38.062 8.815 1.00 25.52 **ATOM** 176 CA THR 178 58.508 38.772 10.064 1.00 18.93 **ATOM** 177 CB THR 178 57.828 38.064 11.258 1.00 21.81 **ATOM** 178 OG1 THR 178 58.348 36.736 11.394 1.00 24.18 **ATOM** 179 CG2 THR 178 56.330 37.971 11.032 1.00 13.81 **ATOM** 180 C THR 178 59.993 38.967 10:358 1.00 20.69 **ATOM** 181 O THR 178 60.373 39.407 11.448 1.00 20.56 **ATOM** 182 N **ASN** 179 60.837 38.645 9.385 1.00 23.68 62.275 38.802 **ATOM 183 CA ASN** 179 9.555 1.00 28.22 **ATOM 184 CB ASN** 179 63.022 37.627 8.927 1.00 27.45 **ATOM 185 CG ASN** 179 64.460 37.529 9.402 1.00 33.98 **ATOM** 65.342 37.131 8.644 1.00 42.72 186 OD1 ASN 179 **ATOM** 187 ND2 ASN 179 64.702 37.865 10.667 1.00 31.14 62.689 40.115 8.902 1.00 34.47 **ATOM** 188 C ASN 179 **ATOM** 189 O **ASN** 179 62.832 40.200 7.678 1.00 36.54 **ATOM** 190 N ALA 180 62.874 41.135 9.735 1.00 37.39 **ATOM** 191 CA ALA 180 63.235 42.479 9.292 1.00 33.71 63.555 43.352 10.494 1.00 31.57 **ATOM** 192 CB ALA 180

ATOM	193 C ALA 180	64.375 42.545 8.284 1.00 37.87
ATOM	194 O ALA 180	65.458 42.018 8.525 1.00 35.26
ATOM	195 N GLN 181	64.095 43.187 7.150 1.00 40.55
ATOM	196 CA GLN 181	65.049 43.391 6.057 1.00 42.95
ATOM	197 CB GLN 181	66.344 44.043 6.570 1.00 45.47
ATOM	198 CG GLN 181	66.144 45.326 7.383 1.00 52.70
ATOM	199 CD GLN 181	65.351 46.399 6.650 1.00 55.03
ATOM	200 OE1 GLN 181	65.270 46.412 5.421 1.00 59.56
ATOM	201 NE2 GLN 181	64.757 47.308 7.411 1.00 54.39
ATOM	202 C GLN 181	65.391 42.176 5.197 1.00 44.27
ATOM	203 O GLN 181	66.181 42.291 4.251 1.00 46.47
ATOM	204 N GLY 182	64.797 41.025 5.508 1.00 42.17
ATOM	205 CA GLY 182	65.054 39.815 4.742 1.00 42.63
ATOM	206 C GLY 182	66.522 39.584 4.427 1.00 47.40
ATOM	207 O GLY 182	67.382 39.691 5.306 1.00 49.38
ATOM	208 N SER 183	66.816 39.297 3.163 1.00 49.46
ATOM	209 CA SER 183	68.189 39.061 2.733 1.00 54.13
ATOM	210 CB SER 183	68.208 38.225 1.449 1.00 55.08
ATOM	211 OG SER 183	67.197 38.647 0.546 1.00 63.54
ATOM	212 C SER 183	68.949 40.369 2.532 1.00 54.84
ATOM	213 O SER 183	70.175 40.373 2.407 1.00 56.90
ATOM	214 N HIS 184	68.223 41.482 2.535 1.00 55.77
ATOM	215 CA HIS 184	68.854 42.775 2.342 1.00 57.78
ATOM	216 C HIS 184	69.605 43.296 3.556 1.00 59.09
ATOM	217 O HIS 184	70.312 44.301 3.454 1.00 60.34
ATOM	218 N TRP 185	69.502 42.597 4.686 1.00 55.60
ATOM	219 CA TRP 185	70.159 43.020 5.923 1.00 53.73
ATOM	220 CB TRP 185	69.973 41.973 7.030 1.00 50.40
ATOM	221 CG TRP 185	70.746 40.694 6.837 1.00 48.09
ATOM ATOM	222 CD2 TRP 185 223 CE2 TRP 185	72.091 40.419 7.269 1.00 47.38
ATOM		72.390 39.094 6.888 1.00 40.29
ATOM	224 CE3 TRP 185 225 CD1 TRP 185	73.071 41.169 7.937 1.00 45.43 70.301 39.554 6.234 1.00 49.87
ATOM	226 NE1 TRP 185	70.301 39.554 6.234 1.00 49.87 71.280 38.589 6.262 1.00 48.02
ATOM	227 CZ2 TRP 185	73.628 38.496 7.154 1.00 38.65
ATOM	228 CZ3 TRP 185	74.304 40.573 8.201 1.00 43.26
ATOM	229 CH2 TRP 185	74.570 39.250 7.807 1.00 40.00
ATOM	230 C TRP 185	71.638 43.386 5.800 1.00 55.99
ATOM	231 O TRP 185	72.089 44.359 6.401 1.00 52.84
ATOM	232 N LYS 186	72.389 42.614 5.021 1.00 59.15
ATOM	233 CA LYS 186	73.818 42.863 4.843 1.00 64.01
ATOM	234 CB LYS 186	74.466 41.688 4.091 1.00 64.67
ATOM	235 CG LYS 186	75.943 41.868 3.729 1.00 65.58
ATOM	236 CD LYS 186	76.817 42.181 4.946 1.00 62.03
ATOM	237 CE LYS 186	78.238 42.512 4.515 1.00 61.52
ATOM	238 NZ LYS 186	78.988 43.243 5.579 1.00 61.67
ATOM	239 C LYS 186	74.131 44.203 4.160 1.00 67.49
		71100 111m00 TILOU 1,00 U/175

ATOM		75.164 44.816 4.432 1.00 68.66
ATOM		73.221 44.678 3.316 1.00 68.99
ATOM	242 CA GLN 187	73.431 45.939 2.612 1.00 69.65
ATOM	243 CB GLN 187	72.880 45.867 1.180 1.00 73.76
ATOM	· · · · · · ·	73.632 44.935 0.237 1.00 78.61
ATOM	245 CD GLN 187	73.368 43.471 0.525 1.00 84.96
ATOM	246 OE1 GLN 187	74.203 42.782 1.109 1.00 87.73
ATOM	247 NE2 GLN 187	72.197 42.989 0.122 1.00 84.98
ATOM	248 C GLN 187	72.817 47.141 3.323 1.00 69.16
ATOM	249 O GLN 187	73.379 48.235 3.299 1.00 71.39
ATOM	250 N ARG 188	71.666 46.936 3.953 1.00 65.82
ATOM	251 CA ARG 188	70.961 48.014 4.639 1.00 65.00
ATOM	252 CB ARG 188	69.458 47.739 4.591 1.00 66.20
ATOM	253 CG ARG 188	68.957 47.483 3.181 1.00 70.30
ATOM	254 CD ARG 188	67.463 47.212 3.132 1.00 78.59
ATOM	255 NE ARG 188	67.003 47.008 1.760 1.00 87.71
ATOM	256 CZ ARG 188	67.011 47.946 0.814 1.00 94.10
ATOM	257 NH1 ARG 188	67.453 49.171 1.081 1.00 97.26
ATOM	258 NH2 ARG 188	66.589 47.657 -0.409 1.00 94.07
ATOM	259 C ARG 188	71.409 48.286 6.077 1.00 65.39
ATOM	260 O ARG 188	70.900 49.201 6.727 1.00 65.20
ATOM	261 N ARG 189	72.372 47.506 6.561 1.00 64.28
ATOM	262 CA ARG 189	72.882 47.654 7.922 1.00 60.75
ATOM	263 CB ARG 189	73.691 46.409 8.321 1.00 56.87
ATOM	264 CG ARG 189	75.050 46.308 7.630 1.00 59.52
ATOM	265 CD ARG 189	75.580 44.891 7.589 1.00 55.86
ATOM	266 NE ARG 189	75.874 44.348 8.907 1.00 55.48
ATOM	267 CZ ARG 189	77.055 43.849 9.257 1.00 61.38
ATOM	268 NH1 ARG 189	78.057 43.832 8.388 1.00 62.54
ATOM	269 NH2 ARG 189	77.225 43.328 10.465 1.00 62.20
ATOM	270 C ARG 189	73.747 48.907 8.082 1.00 60.91
ATOM	271 O ARG 189	74.548 49.245 7.207 1.00 60.67
ATOM	272 N LYS 190	73.575 49.591 9.207 1.00 59.06
ATOM	273 CA LYS 190	74.340 50.790 9.521 1.00 55.00
ATOM	274 CB LYS 190	73.423 52.008 9.582 1.00 55.45
ATOM	275 C LYS 190	74.991 50.542 10.875 1.00 51.52
ATOM	276 O LYS 190	74.320 50.144 11.830 1.00 51.68
ATOM	277 N PHE 191	76.304 50.721 10.944 1.00 50.49
ATOM	278 CA PHE 191	77.037 50.508 12.186 1.00 50.17
ATOM	279 CB PHE 191	78.546 50.571 11.943 1.00 48.38
ATOM	280 CG PHE 191	79.090 49.423 11.142 1.00 49.66
ATOM	281 CD1 PHE 191	78.873 49.348 9.768 1.00 51.03
ATOM	282 CD2 PHE 191	79.845 48.429 11.759 1.00 46.28
ATOM	283 CE1 PHE 191	79.403 48.298 9.018 1.00 51.35
ATOM	284 CE2 PHE 191	80.379 47.377 11.021 1.00 47.26
ATOM	285 CZ PHE 191	80.158 47.311 9.646 1.00 48.48
ATOM	286 C PHE 191	76.663 51.534 13.248 1.00 48.61

ATOM 287 O PHE 191 76.507 52.720 12.952 1.00 50.38 **ATOM** 288 N LEU 192 76.488 51.068 14.479 1.00 47.31 **ATOM 289 CA LEU** 192 76.169 51.958 15.584 1.00 42.72 **ATOM** 290 CB LEU 192 75.845 51.151 16.844 1.00 36.66 **ATOM** 291 CG LEU 192 75.397 51.949 18.068 1.00 31.01 **ATOM** 292 CD1 LEU 192 74.048 52.590 17.786 1.00 28.37 **ATOM** 293 CD2 LEU 192 75.318 51.043 19.289 1.00 29.60 **ATOM** 294 C LEU 192 77.447 52.760 15.800 1.00 42.28 **ATOM** 295 O LEU 192 78.528 52.179 15.932 1.00 39.71 **ATOM** 296 N **PRO** 193 77.350 54.104 15.781 1.00 45.15 **ATOM** 297 CD PRO 193 76.095 54.865 15.617 1.00 43.82 **ATOM** 298 CA PRO 193 78.493 55.006 15.973 1.00 43.14 ATOM 299 CB PRO 193 77.820 56.306 16.400 1.00 44.37 **ATOM** 300 CG PRO 193 76.571 56.308 15.565 1.00 41.66 **ATOM** 301 C 193 **PRO** 79.476 54.498 17.028 1.00 43.34 **ATOM** 302 O **PRO** 193 79.103 54.296 18.182 1.00 45.18 **ATOM** 303 N ASP 194 80.732 54.317 16.628 1.00 44.22 **ATOM** 304 CA ASP 194 81.781 53.804 17.512 1.00 47.20 **ATOM** 305 CB ASP 194 83.108 53.732 16.761 1.00 41.89 **ATOM** 306 C **ASP** 194 81.962 54.511 18.866 1.00 51.99 **ATOM** 307 O **ASP** 194 82.636 53.986 19.752 1.00 54.04 **ATOM ASP** 308 N 195 81.381 55.698 19.025 1.00 55.21 **ATOM** 309 CA ASP 195 81.489 56.428 20.288 1.00 57.50 **ATOM** 310 CB ASP 195 81.423 57.948 20.061 1.00 60.04 **ATOM** 311 CG ASP 195 80.123 58.398 19.406 1.00 68.39 **ATOM** 312 OD1 ASP 195 79.211 58.847 20.136 1.00 69.46 **ATOM** 313 OD2 ASP 195 80.020 58.322 18.162 1.00 72.91 **ATOM** 314 C ASP 195 80.410 55.976 21.280 1.00 58.05 **ATOM ASP** 195 315 O 80.540 56.180 22.491 1.00 58.97 ATOM 196 79.349 55.363 20.759 1.00 56.06 316 N ILE **ATOM** 317 CA ILE 196 78.247 54.863 21.580 1.00 50.48 **ATOM** 318 CB ILE 196 76.930 54.762 20.766 1.00 45.82 319 CG2 ILE **ATOM** 196 75.818 54.166 21.621 1.00 44.04 **ATOM** 320 CG1 ILE 196 76.517 56.147 20.261 1.00 44.27 **ATOM** 321 CD1 ILE 196 75.179 56.171 19.541 1.00 45.25 **ATOM** 322 C ILE 196 78.603 53.484 22.135 1.00 47.66 **ATOM** 323 O ILE 196 79.138 52.636 21.419 1.00 43.96 **ATOM** 324 N **GLY** 197 78.309 53.269 23.414 1.00 46.29 325 CA GLY **ATOM** 197 78.608 51.995 24.045 1.00 48.03 **ATOM** 326 C **GLY** 197 79.978 51.963 24.692 1.00 50.42 **ATOM** 327 O **GLY** 197 80.463 50.902 25.070 1.00 46.66 **GLN ATOM** 328 N 198 80.583 53.137 24.854 1.00 56.94 **ATOM 329 CA GLN** 198 81.910 53.259 25.454 1.00 59.51 **ATOM** 330 CB GLN 198 82.751 54.257 24.649 1.00 62.53 **ATOM 331 CG GLN** 198 83.232 53.718 23.316 1.00 69.39 **ATOM** 332 CD GLN 198 84.088 52.484 23.483 1.00 76.76 **ATOM** 333 OE1 GLN 83.745 51.399 22.996 1.00 81.73 198

334 NE2 GLN 198 **ATOM** 85.205 52.632 24.192 1.00 78.09 **ATOM** 335 C GLN -198 81.915 53.678 26.922 1.00 57.56 **ATOM** 336 O **GLN** 198 82.946 53.584 27.588 1.00 57.71 **ATOM** 337 N SER 199 80.770 54.128 27.425 1.00 54.11 **ATOM** 338 CA SER 199 80.676 54.600 28.800 1.00 46.28 **ATOM** 339 CB SER 199 80.243 56.067 28.777 1.00 50.28 **ATOM** 340 OG SER 199 80.935 56.776 27.757 1.00 50.95 **ATOM** 341 C **SER** 199 79.776 53.805 29.757 1.00 40.19 **ATOM** 342 O SER 199 78.680 54.252 30.102 1.00 39.26 **ATOM** 343 N PRO 200 80.236 52.629 30.214 1.00 35.63 **ATOM** 344 CD PRO 200 81.530 52.011 29.904 1.00 34.88 **ATOM** 345 CA PRO 200 79.464 51.789 31.139 1.00 37.54 **ATOM** 346 CB PRO 200 80.223 50.457 31.124 1.00 29.86 **ATOM** 347 CG PRO 200 81.207 50.570 29.995 1.00 34.29 **ATOM** 348 C PRO 200 79.521 52.416 32.532 1.00 44.63 **ATOM** 349 O PRO 200 80.443 52.137 33.300 1.00 47.80 **ATOM** 350 N ILE 201 78.532 53.241 32.867 1.00 49.57 201 **ATOM 351 CA ILE** 78.525 53.924 34.158 1.00 49.15 **ATOM** 352 CB ILE 201 78.213 55.426 33.990 1.00 49.19 **ATOM** 353 CG2 ILE 201 78.429 56.150 35.306 1.00 53.37 **ATOM** 354 CG1 ILE 201 79.137 56.037 32.934 1.00 52.55 **ATOM** 355 CD1 ILE 201 78.811 57.471 32.586 1.00 55.26 **ATOM** 356 C ILE 201 77.625 53.352 35.254 1.00 49.88 **ATOM** 357 O ILE 201 78.044 53.250 36.408 1.00 50.20 **ATOM** 358 N VAL 202 76.384 53.014 34.920 1.00 47.85 **ATOM** 359 CA VAL 202 75.468 52.474 35.927 1.00 45.76 **ATOM** 360 CB VAL 202 74.015 52.415 35.400 1.00 39.98 **ATOM** 361 CG1 VAL 202 73.072 51.896 36.482 1.00 35.94 **ATOM** 362 CG2 VAL 202 73.574 53.799 34.944 1.00 29.43 **ATOM** 363 C VAL 202 75.954 51.093 36.373 1.00 50.57 **ATOM** VAL 202 364 O 76.296 50.249 35.545 1.00 49.50 **ATOM** 365 N SER 203 76.009 50.876 37.683 1.00 54.82 **ATOM** 366 CA SER 203 76.490 49.609 38.223 1.00 59.26 **ATOM 367 CB SER** 203 77.067 49.809 39.628 1.00 64.88 203 **ATOM** 368 OG SER 76.127 50.428 40.492 1.00 75.47 **ATOM** 369 C SER 203 75.457 48.491 38.244 1.00 55.78 **ATOM** 370 O SER 203 74.285 48.712 38.544 1.00 57.50 **ATOM** MET 204 371 N 75.923 47.283 37.958 1.00 52.29 **372 CA MET** 204 **ATOM** 75.076 46.103 37.948 1.00 50.42 **ATOM 373 CB MET** 204 75.032 45.487 36.548 1.00 47.74 **ATOM 374 CG MET** 204 74.243 46.297 35.541 1.00 43.40 **375 SD MET ATOM** 204 72.491 46.348 35.953 1.00 40.93 **ATOM** 376 CE MET 204 71.947 44.785 35.241 1.00 39.19 **ATOM** 377 C 75.670 45.107 38.925 1.00 49.42 MET 204 **ATOM** 378 O 204 MET 76.892 45.020 39.062 1.00 52.25 **ATOM** 379 N PRO 205 74.816 44.329 39.605 1.00 47.73 **ATOM** 73.344 44.414 39.549 1.00 48.94 380 CD PRO 205

ATOM 381 CA PRO 205 75.250 43.326 40.580 1.00 47.34 382 CB PRO **ATOM** 205 73.982 42.513 40.810 1.00 49.44 **ATOM** 383 CG PRO 205 72.907 43.562 40.725 1.00 50.62 **ATOM** 384 C **PRO** 205 76.431 42.442 40.168 1.00 47.12 385 O ATOM **PRO** 205 77.299 42.160 40.990 1.00 51.21 **ATOM** 386 N- ASP 206 76.487 42.023 38.909 1.00 48.81 387 CA ASP **ATOM** 206 77.583 41.160 38.465 1.00 49.88 **ATOM** 388 CB ASP 206 77.128 40.223 37.330 1.00 54.06 **ATOM** 389 CG ASP 206 76.598 40.967 36.107 1.00 57.34 **ATOM** 390 OD1 ASP 206 77.056 42.095 35.811 1.00 52.21 **ATOM** 391 OD2 ASP 206 75.719 40.397 35.423 1.00 59.16 **ATOM** 392 C **ASP** 206 78.902 41.843 38.093 1.00 48.70 **ATOM** 393 O **ASP** 206 79.862 41.171 37.715 1.00 49.75 **ATOM** 394 N GLY 207 78.946 43.168 38.161 1.00 47.54 **ATOM** 395 CA GLY 207 80.174 43.869 37.820 1.00 49.23 **ATOM** 396 C **GLY** 207 80.169 44.585 36.482 1.00 51.96 **ATOM** 397 O **GLY** 207 80.783 45.645 36.348 1.00 56.32 **ATOM** 398 N **ASP** 208 79.510 44.005 35.481 1.00 52.50 **ATOM** 399 CA ASP 208 79.435 44.624 34.157 1.00 48.00 **ATOM** 400 CB ASP 208 78.968 43.609 33.115 1.00 53.23 **ATOM** 401 CG ASP 208 80.038 42.592 32.774 1.00 53.17 **ATOM** 402 OD1 ASP 208 81.130 43.006 32.335 1.00 57.42 **ATOM** 403 OD2 ASP 208 79.787 41.380 32.942 1.00 55.64 **ATOM** 404 C ASP 208 78.497 45.823 34.187 1.00 46.68 **ATOM** 405 O ASP 208 77.283 45.671 34.332 1.00 45.81 **ATOM** 406 N LYS 209 79.075 47.014 34.077 1.00 45.95 **ATOM** 407 CA LYS 209 78.313 48.257 34.115 1.00 45.87 **ATOM** 408 CB LYS 209 79.235 49.418 34.478 1.00 46.90 **ATOM** 409 C LYS 209 77.561 48.546 32.812 1.00 41.17 LYS 209 **ATOM** 410 O 77.951 48.074 31.745 1.00 39.51 **ATOM** 411 N VAL 210 76.500 49.344 32.916 1.00 39.35 412 CA VAL **ATOM** 210 75.652 49.713 31.782 1.00 38.03 **ATOM** 413 CB VAL 210 74.136 49.584 32.140 1.00 32.13 **ATOM** 414 CG1 VAL 210 73.269 49.926 30.937 1.00 27.92 **ATOM** 415 CG2 VAL 210 73.818 48.183 32.627 1.00.29.43 **ATOM** VAL 210 416 C 75.895 51.134 31.263 1.00 38.68 **ATOM** VAL 417 O 210 76.090 52.079 32.038 1.00 39.57 **ATOM** 418 N ASP 211 75.848 51.272 29.942 1.00 39.19 **ATOM** 419 CA ASP 211 76.019 52.544 29.254 1.00 38.39 ATOM 420 CB ASP 211 76.794 52.327 27.946 1.00 40.36 **ATOM** 421 CG ASP 211 77.051 53.620 27.177 1.00 36.85 **ATOM** 422 OD1 ASP 211 76.193 54.528 27.167 1.00 37.95 **ATOM** 423 OD2 ASP 211 78.121 53.716 26.553 1.00 33.87 **ATOM** 424 C ASP 211 74.601 53.040 28.958 1.00 40.60 425 O **ATOM** ASP 211 73.919 52.517 28.073 1.00 40.36 **ATOM** 426 N LEU 212 74.185 54.074 29.680 1.00 41.55 72.854 54.664 29.552 1.00 38.39 **ATOM** 427 CA LEU 212

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ATOM	428 CB LEU 212	72.759 55.883 30.467 1.00 40.93
ATOM	429 CG LEU 212	71.575 55.979 31.428 1.00 45.32
ATOM	430 CD1 LEU 212	71.271 54.626 32.047 1.00 43.83
ATOM	431 CD2 LEU 212	71.900 57.007 32.502 1.00 44.93
ATOM	432 C LEU 212	72.448 55.050 28.133 1.00 37.61
ATOM	433 O LEU 212	71.318 54.805 27.719 1.00 33.71
ATOM	434 N GLU 213	73.360 55.670 27.393 1.00 41.23
ATOM	435 CA GLU 213	73.068 56.084 26.023 1.00 43.48
ATOM	436 CB GLU 213	74.181 56.986 25.481 1.00 47.66
ATOM	437 CG GLU 213	73.919 57.494 24.065 1.00 56.87
ATOM	438 CD GLU 213	75.121 58.180 23.433 1.00 60.87
ATOM	439 OE1 GLU 213	76.258 57.996 23.924 1.00 60.37
ATOM	440 OE2 GLU 213	74.921 58.894 22.423 1.00 61.13
ATOM	441 C GLU 213	72.889 54.880 25.102 1.00 39.29
ATOM	442 O GLU 213	71.965 54.841 24.290 1.00 36.66
ATOM	443 N ALA 214	73.785 53.906 25.233 1.00 36.33
ATOM	444 CA ALA 214	73.739 52.693 24.422 1.00 34.89
ATOM	445 CB ALA 214	74.946 51.817 24.711 1.00 30.70
ATOM	446 C ALA 214	72.454 51.938 24.718 1.00 31.96
ATOM	447 O ALA 214	71.739 51.523 23.804 1.00 33.93
ATOM	448 N PHE 215	72.151 51.798 26.003 1.00 28.47
ATOM	449 CA PHE 215	70.947 51.116 26.445 1.00 29.74
ATOM	450 CB PHE 215	70.819 51.223 27.962 1.00 23.73
ATOM	451 CG PHE 215	69.589 50.568 28.515 1.00 22.71
ATOM	452 CD1 PHE 215	69.603 49.220 28.858 1.00 22.53
ATOM	453 CD2 PHE 215	68.423 51.301 28.712 1.00 19.74
ATOM	454 CE1 PHE 215	68.477 48.606 29.391 1.00 20.75
ATOM	455 CE2 PHE 215	67.290 50.698 29.245 1.00 21.02
ATOM	456 CZ PHE 215	67.318 49.346 29.586 1.00 19.50
ATOM	457 C PHE 215	69.730 51.742 25.771 1.00 34.64
ATOM	458 O PHE 215	68.872 51.034 25.239 1.00 39.86
ATOM	459 N SER 216	69.677 53.071 25.771 1.00 34.78
ATOM	460 CA SER 216	68.572 53.801 25.160 1.00 36.01
ATOM	461 CB SER 216	68.762 55.302 25.366 1.00 37.36
ATOM	462 OG SER 216	67.537 55.987 25.193 1.00 48.33
ATOM	463 C SER 216	68.458 53.475 23.664 1.00 37.06
ATOM	464 O SER 216	67.358 53.250 23.148 1.00 33.23
ATOM	465 N GLU 217	69.601 53.410 22.986 1.00 36.25
ATOM	466 CA GLU 217	69.645 53.091 21.562 1.00 36.99
ATOM	467 CB GLU 217	71.092 53.104 21.064 1.00 37.10
ATOM	468 CG GLU 217	71.682 54.491 20.912 1.00 44.30
ATOM	469 CD GLU 217	71.016 55.284 19.802 1.00 51.30
ATOM	470 OE1 GLU 217	71.439 55.142 18.633 1.00 57.25
ATOM	471 OE2 GLU 217	70.070 56.046 20.096 1.00 52.50
ATOM	472 C GLU 217	69.019 51.726 21.286 1.00 36.93
ATOM	473 O GLU 217	68.191 51.577 20.381 1.00 41.06
ATOM	474 N PHE 218	69.395 50.740 22.093 1.00 30.27

ATOM	475 CA PHE 218	68.875 49.388 21.947 1.00 27.20
ATOM	476 CB PHE 218	69.679 48.421 22.814 1.00 28.10
ATOM	477 CG PHE 218	71.124 48.330 22.428 1.00 24.84
ATOM	478 CD1 PHE 218	72.117 48.286 23.398 1.00 21.78
ATOM	479 CD2 PHE 218	71.495 48.301 21.087 1.00 24.78
ATOM	480 CE1 PHE 218	73.458 48.215 23.040 1.00 24.08
ATOM	481 CE2 PHE 218	72.834 48.230 20.719 1.00 25.33
ATOM	482 CZ PHE 218	73.818 48.187 21.697 1.00 25.04
ATOM	483 C PHE 218	67.381 49.281 22.261 1.00 28.23
ATOM	484 O PHE 218	66.639 48.605 21.543 1.00 33.52
ATOM	485 N THR 219	66.927 49.961 23.310 1.00 27.24
ATOM	486 CA THR 219	65.515 49.913 23.666 1.00 29.28
ATOM	487 CB THR 219	65.238 50.533 25.052 1.00 30.97
ATOM	488 OG1 THR 219	65.724 51.880 25.090 1.00 35.50
ATOM	489 CG2 THR 219	65.901 49.712 26.149 1.00 30.78
ATOM	490 C THR 219	64.660 50.612 22.615 1.00 33.29
ATOM	491 O THR 219	63.473 50.317 22.474 1.00 36.85
ATOM	492 N LYS 220	65.276 51.515 21.860 1.00 35.23
ATOM	493 CA LYS 220	64.579 52.253 20.816 1.00 38.97
ATOM	494 CB LYS 220	65.506 53.334 20.236 1.00 44.67
ATOM	495 CG LYS 220	64.805 54.491 19.513 1.00 58.02
ATOM	496 CD LYS 220	64.406 54.130 18.079 1.00 68.57
ATOM	497 CE LYS 220	63.732 55.296 17.347 1.00 70.50
ATOM	498 NZ LYS 220	62.395 55.668 17.905 1.00 66.08
ATOM	499 C LYS 220	64.112 51.289 19.721 1.00 38.48
ATOM	500 O LYS 220	63.021 51.446 19.173 1.00 37.18
ATOM	501 N ILE 221	64.917 50.270 19.432 1.00 36.19
ATOM	502 CA ILE 221	64.563 49.305 18.394 1.00 36.77
ATOM	503 CB ILE 221	65.756 48.996 17.457 1.00 34.41
ATOM	504 CG2 ILE 221	66.270 50.276 16.814 1.00 38.54
ATOM	505 CG1 ILE 221	66.864 48.267 18.221 1.00 32.93
ATOM	506 CD1 ILE 221	67.984 47.752 17.338 1.00 31.12
ATOM	507 C ILE 221	64.002 47.971 18.888 1.00 38.22
ATOM	508 O ILE 221	63.499 47.181 18.089 1.00 38.90
ATOM	509 N ILE 222	64.048 47.719 20.191 1.00 35.75
ATOM	510 CA ILE 222	63.557 46.446 20.702 1.00 31.77
ATOM	511 CB ILE 222	64.086 46.152 22.130 1.00 33.14
		63.203 46.813 23.183 1.00 24.60
		64.147 44.638 22.350 1.00 32.60
		64.860 44.226 23.609 1.00 34.52
ATOM	515 C ILE 222	62.042 46.240 20.624 1.00 32.56
ATOM	516 O ILE 222	61.581 45.109 20.452 1.00 35.74
ATOM	517 N THR 223	61.262 47.313 20.720 1.00 29.43
		59.806 47.170 20.651 1.00 33.57
	519 CB THR 223	59.075 48.514 20.903 1.00 38.99
ATOM		59.422 49.010 22.205 1.00 41.23
ATOM	521 CG2 THR 223	57.558 48.325 20.836 1.00 36.98

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ATOM	522 C THR 223	59.355 46.528 19.325 1.00 31.45
ATOM	523 O THR 223	58.571 45.571 19.334 1.00 26.77
ATOM	524 N PRO 224	59.824 47.054 18.173 1.00 31.35
ATOM	525 CD PRO 224	60.570 48.306 17.950 1.00 30.11
ATOM	526 CA PRO 224	59.424 46.462 16.891 1.00 30.38
ATOM	527 CB PRO 224	60.149 47.336 15.865 1.00 30.09
ATOM	528 CG PRO 224	60.200 48.659 16.530 1.00 31.86
ATOM	529 C PRO 224	59.882 45.007 16.795 1.00 29.51
ATOM	530 O PRO 224	59.147 44.153 16.295 1.00 32.52
ATOM	531 N ALA 225	61.090 44.734 17.285 1.00 32.63
ATOM	532 CA ALA 225	61.650 43.385 17.268 1.00 22.63
ATOM	533 CB ALA 225	
ATOM	534 C ALA 225	
ATOM		60.752 42.416 18.026 1.00 23.53
		60.455 41.323 17.544 1.00 25.07
ATOM		60.296 42.828 19.202 1.00 22.61
ATOM	537 CA ILE 226	59.420 41.989 20.007 1.00 19.46
ATOM	538 CB ILE 226	59.120 42.644 21.360 1.00 20.25
ATOM	539 CG2 ILE 226	58.071 41.843 22.105 1.00 16.75
ATOM	540 CG1 ILE 226	60.401 42.772 22.182 1.00 19.30
ATOM	541 CD1 ILE 226	60.240 43.645 23.413 1.00 20.92
ATOM	542 C ILE 226	58.112 41.768 19.251 1.00 21.28
ATOM	543 O ILE 226	57.553 40.670 19.256 1.00 23.75
ATOM	544 N THR 227	57.629 42.821 18.598 1.00 24.46
ATOM	545 CA THR 227	56.393 42.752 17.826 1.00 25.81
ATOM	546 CB THR 227	56.020 44.136 17.260 1.00 31.00
ATOM	547 OG1 THR 227	55.772 45.039 18.345 1.00 35.43
ATOM	548 CG2 THR 227	54.776 44.049 16.388 1.00 29.01
ATOM	549 C THR 227	56.508 41.728 16.691 1.00 22.85
ATOM	550 O THR 227	55.589 40.939 16.469 1.00 22.84
ATOM ATOM	551 N ARG 228	57.647 41.713 16.004 1.00 16.09
	552 CA ARG 228	57.862 40.765 14.919 1.00 16.97
ATOM	553 CB ARG 228	59.161 41.064 14.174 1.00 14.71
ATOM	554 CG ARG 228	59.137 42.369 13.391 1.00 16.22
ATOM ATOM	555 CD ARG 228	60.309 42.447 12.422 1.00 20.90
	556 NE ARG 228 557 CZ ARG 228	61.595 42.207 13.078 1.00 24.94
ATOM		62.243 43.113 13.805 1.00 35.06
ATOM	558 NH1 ARG 228	61.729 44.328 13.973 1.00 36.35
ATOM	559 NH2 ARG 228	63.404 42.807 14.370 1.00 32.78
ATOM	560 C ARG 228	57.866 39.326 15.431 1.00 21.63
ATOM	561 O ARG 228	57.477 38.407 14.704 1.00 24.47
ATOM	562 N VAL 229	58.304 39.128 16.675 1.00 20.00
ATOM	563 CA VAL 229	58.319 37.793 17.266 1.00 18.39
ATOM	564 CB VAL 229	59.103 37.745 18.606 1.00 19.20
ATOM	565 CG1 VAL 229	58.938 36.382 19.265 1.00 14.19
ATOM	566 CG2 VAL 229	60.581 38.001 18.356 1.00 14.81
ATOM	567 C VAL 229	56.875 37.367 17.501 1.00 20.00
ATOM	568 O VAL 229	56.499 36.227 17.212 1.00 20.04

ATOM 569 N VAL 230 56.058 38.291 18.003 1.00 19.60 **ATOM** 570 CA VAL 230 54.651 37.996 18.247 1.00 18.72 **ATOM** 571 CB VAL 230 53.930 39.185 18.912 1.00 22.15 **ATOM** 572 CG1 VAL 230 52.452 38.862 19.113 1.00 15.66 ATOM 573 CG2 VAL 230 54.592 39.522 20.248 1.00 21.05 **ATOM** 574 C VAL 230 53.967 37.660 16.917 1.00 26.17 **ATOM** 575 O VAL 230 53.188 36.704 16.836 1.00 28.01 **ATOM ASP** 576 N 231 54.288 38.426 15.873 1.00 25.07 **ATOM** 577 CA ASP 231 53.714 38.216 14.542 1.00 26.10 **ATOM** 578 CB ASP 231 54.169 39.309 13.568 1.00 22.15 **ATOM 579 CG ASP** 231 53.620 40.684 13.921 1.00 29.49 **ATOM** 580 OD1 ASP 231 52.587 40.767 14.624 1.00 30.93 **ATOM** 581 OD2 ASP 231 54.223 41.687 13.481 1.00 31.74 **ATOM** 582 C **ASP** 231 54.087 36.842 13.989 1.00 27.35 **ATOM** 583 O **ASP** 231 53.245 36.154 13.408 1.00 25.89 **ATOM** 584 N PHE 232 55.347 36.451 14.175 1.00 24.29 **ATOM** 585 CA PHE 232 55.825 35.154 13.714 1.00 22.90 **ATOM 586 CB PHE** 57.302 34.956 14.090 1.00 20.56 232 **ATOM 587 CG PHE** 232 57.762 33.525 14.007 1.00 24.20 588 CD1 PHE **ATOM** 232 57.952 32.910 12.772 1.00 23.44 **ATOM** 589 CD2 PHE 232 57.959 32.776 15.167 1.00 19.41 **ATOM** 590 CE1 PHE 232 58.329 31.567 12.689 1.00 19.53 **ATOM** 591 CE2 PHE 232 58.336 31.431 15.100 1.00 21.09 **ATOM** 592 CZ PHE 232 58.520 30.824 13.858 1.00 21.61 **ATOM** 593 C PHE 232 54.984 34.047 14.341 1.00 24.18 **ATOM** 594 O PHE 232 54.481 33.160 13.645 1.00 22.26 **ATOM** 595 N ALA 233 54.810 34.127 15.656 1.00 23.90 596 CA ALA 233 **ATOM** 54.048 33.128 16.397 1.00 22.60 **ATOM** 597 CB ALA 233 54.088 33.435 17.890 1.00 15.34 598 C ALA **ATOM** 233 52.609 33.040 15.917 1.00 22.04 **ATOM** ALA 599 O 233 52.084 31.948 15.697 1.00 22.86 **ATOM** 600 N LYS 234 51.978 34.195 15.743 1.00 25.04 **ATOM** 601 CA LYS 234 50.593 34.248 15.298 1.00 27.68 **ATOM** 602 CB LYS 234 50.096 35.691 15.292 1.00 31.41 **ATOM** 603 CG LYS 234 49.845 36.248 16.682 1.00 40.37 **ATOM** 604 CD LYS 234 49.212 37.626 16.604 1.00 57.53 **ATOM** 605 CE LYS 234 48.772 38.112 17.974 1.00 64.28 **ATOM** 606 NZ LYS 234 48.164 39.473 17.904 1.00 67.19 **ATOM** 607 C LYS 234 50.358 33.588 13.939 1.00 26.42 **ATOM** 608 O LYS 234 49.269 33.067 13.674 1.00 31.34 **ATOM** 609 N LYS 235 51.382 33.588 13.093 1.00 24.38 **ATOM** 610 CA LYS 235 51.278 32.985 11.770 1.00 26.42 **ATOM** 611 CB LYS 235 52.244 33.664 10.805 1.00 24.92 **ATOM** 612 CG LYS 235 51.908 35.127 10.583 1.00 22.41 **ATOM** 613 CD LYS 235 52.843 35.775 9.588 1.00 29.38 **ATOM** 614 CE LYS 235 52.481 37.234 9.395 1.00 33.49 **ATOM** 615 NZ LYS 235 53.354 37.869 8.376 1.00 40.13

ATOM	616 C LYS 235	51.470 31.469 11.759 1.00 30.02
ATOM	617 O LYS 235	51.417 30.838 10.699 1.00 30.37
ATOM	618 N LEU 236	51.722 30.889 12.930 1.00 32.39
ATOM	619 CA LEU 236	51.878 29.443 13.053 1.00 36.24
ATOM	620 CB LEU 236	52.944 29.080 14.089 1.00 29.91
ATOM	621 CG LEU 236	54.373 29.516 13.765 1.00 24.69
ATOM	622 CD1 LEU 236	55.299 29.054 14.877 1.00 22.71
ATOM	623 CD2 LEU 236	54.811 28.942 12.427 1.00 24.48
ATOM	624 C LEU 236	50.520 28.891 13.470 1.00 41.22
ATOM	625 O LEU 236	49.936 29.333 14.467 1.00 41.45
ATOM	626 N PRO 237	50.012 27.895 12.729 1.00 47.86
ATOM	627 CD PRO 237	50.739 27.190 11.657 1.00 49.32
ATOM	628 CA PRO 237	48.713 27.262 12.992 1.00 50.28
ATOM	629 CB PRO 237	48.669 26.128 11.962 1.00 55.25
ATOM	630 CG PRO 237	50.135 25.818 11.706 1.00 54.08
ATOM	631 C PRO 237	48.495 26.751 14.422 1.00 47.94
ATOM	632 O PRO 237	47.533 27.134 15.087 1.00 42.48
ATOM	633 N MET 238	49.415 25.927 14.906 1.00 49.51
ATOM	634 CA MET 238	49.306 25.354 16.245 1.00 53.49
ATOM	635 CB MET 238	50.379 24.275 16.424 1.00 52.52
ATOM	636 CG MET 238	50.028 22.959 15.728 1.00 56.00
ATOM	637 SD MET 238	51.443 21.961 15.204 1.00 50.16
ATOM	638 CE MET 238	50.896 21.440 13.552 1.00 55.71
ATOM	639 C MET 238	49.352 26.362 17.395 1.00 54.20
ATOM	640 O MET 238	48.930 26.058 18.515 1.00 54.72
ATOM	641 N PHE 239	49.803 27.578 17.101 1.00 50.11
ATOM	642 CA PHE 239	49.917 28.619 18.117 1.00 41.11
ATOM	643 CB PHE 239	51.089 29.552 17.788 1.00 34.80
ATOM	644 CG PHE 239	51.336 30.607 18.826 1.00 30.25
ATOM	645 CD1 PHE 239	52.127 30.332 19.937 1.00 25.66
ATOM	646 CD2 PHE 239	50.786 31.878 18.690 1.00 26.30
ATOM	647 CE1 PHE 239	52.368 31.307 20.896 1.00 30.28
ATOM	648 CE2 PHE 239	51.019 32.862 19.644 1.00 30.49
ATOM	649 CZ PHE 239	51.813 32.576 20.750 1.00 29.00
ATOM	650 C PHE 239	48.647 29.434 18.337 1.00 35.65
ATOM	651 O PHE 239	48.151 29.521 19.457 1.00 30.27
ATOM	652 N SER 240	48.133 30.037 17.272 1.00 36.49
ATOM		46.936 30.866 17.359 1.00 36.37
ATOM	654 CB SER 240	46.622 31.466 15.994 1.00 35.87
ATOM	655 C SER 240	45.707 30.145 17.936 1.00 40.37
ATOM	656 O SER 240	44.784 30.789 18.438 1.00 37.47
ATOM	657 N GLU 241	45.713 28.814 17.889 1.00 43.00
ATOM	658 CA GLU 241	44.605 28.004 18.404 1.00 46.31
ATOM	659 CB GLU 241	44.714 26.566 17.881 1.00 55.84
ATOM	660 CG GLU 241	44.750 26.422 16.360 1.00 69.03
ATOM	661 CD GLU 241	45.141 25.015 15.900 1.00 74.99
ATOM	662 OE1 GLU 241	45.835 24.299 16.658 1.00 77.81

ATOM	663 OE2 GLU 241	44.765 24.629 14.770 1.00 70.58
ATOM	664 C GLU 241	44.587 27.961 19.933 1.00 42.60
ATOM	665 O GLU 241	43.541 27.740 20.545 1.00 43.23
ATOM	666 N LEU 242	45.762 28.125 20.535 1.00 39.31
ATOM	667 CA LEU 242	45.926 28.086 21.987 1.00 34.54
ATOM	668 CB LEU 242	47.417 28.109 22.344 1.00 28.35
ATOM	669 CG LEU 242	48.311 26.974 21.853 1.00 27.59
ATOM	670 CD1 LEU 242	49.750 27.307 22.180 1.00 20.72
ATOM	671 CD2 LEU 242	47.902 25.661 22.500 1.00 24.97
ATOM	672 C LEU 242	45.242 29.240 22.711 1.00 32.23
ATOM	673 O LEU 242	44.956 30.282 22.119 1.00 31.50
ATOM	674 N PRO 243	44.954 29.060 24.010 1.00 34.39
ATOM	675 CD PRO 243	45.118 27.843 24.827 1.00 31.68
ATOM	676 CA PRO 243	44.309 30.134 24.773 1.00 34.39
ATOM	677 CB PRO 243	44.092 29.498 26.154 1.00 32.34
ATOM	678 CG PRO 243	44.081 28.026 25.892 1.00 33.80
ATOM	679 C PRO 243	45.300 31.303 24.873 1.00 35.56
ATOM	680 O PRO 243	46.517 31.082 24.897 1.00 34.99
ATOM	681 N CYS 244	44.791 32.532 24.946 1.00 34.23
ATOM	682 CA CYS 244	45.648 33.714 25.062 1.00 37.03
ATOM	683 CB CYS 244	44.820 34.960 25.376 1.00 43.49
ATOM	684 SG CYS 244	43.820 35.531 24.007 1.00 71.28
ATOM	685 C CYS 244	46.716 33.555 26.135 1.00 34.99
ATOM	686 O CYS 244	47.894 33.802 25.882 1.00 37.49
ATOM	687 N GLU 245	46.305 33.125 27.326 1.00 33.03
ATOM	688 CA GLU 245	47.249 32.944 28.424 1.00 35.72
ATOM	689 CB GLU 245	46.559 32.469 29.716 1.00 37.85
ATOM	690 CG GLU 245	45.294 31.633 29.549 1.00 46.81
ATOM	691 CD GLU 245	44.029 32.478 29.480 1.00 44.81
ATOM	692 OE1 GLU 245	43.606 33.012 30.527 1.00 33.05
ATOM	693 OE2 GLU 245	43.454 32.599 28.377 1.00 48.22
ATOM	694 C GLU 245	48.414 32.035 28.047 1.00 32.29
ATOM	695 O GLU 245	49.558 32.319 28.399 1.00 35.92
ATOM	696 N ASP 246	48.134 30.975 27.295 1.00 30.64
ATOM	697 CA ASP 246	49.182 30.058 26.855 1.00 28.23
ATOM	698 CB ASP 246	48.575 28.809 26.208 1.00 30.51
ATOM	699 CG ASP 246	48.213 27.737 27.222 1.00 33.18
ATOM	700 OD1 ASP 246	48.265 28.006 28.439 1.00 31.26
ATOM	701 OD2 ASP 246	47.884 26.613 26.796 1.00 33.85
ATOM	702 C ASP 246	50.104 30.757 25.860 1.00 30.10
ATOM	703 O ASP 246	51.330 30.651 25.950 1.00 27.08
ATOM	704 N GLN 247	49.500 31.477 24.918 1.00 30.39
ATOM	705 CA GLN 247	50.249 32.208 23.901 1.00 29.08
ATOM	706 CB GLN 247	49.295 32.949 22.964 1.00 27.34
ATOM	707 CG GLN 247	48.390 32.034 22.147 1.00 28.95
ATOM	708 CD GLN 247	47.531 32.796 21.153 1.00 30.74
ATOM	709 OE1 GLN 247	47.850 33.918 20.767 1.00 33.23
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ATOM	710 NE2 GLN 247	46.439 32.185 20.729 1.00 35.19
ATOM	711 C GLN 247	51.190 33.196 24.575 1.00 27.51
ATOM	712 O GLN 247	52.377 33.261 24.256 1.00 28.70
ATOM	713 N ILE 248	50.661 33.921 25.552 1.00 27.81
ATOM	714 CA ILE 248	51.431 34.908 26.295 1.00 29.41
ATOM	715 CB ILE 248	50.525 35.662 27.303 1.00 28.96
ATOM	716 CG2 ILE 248	51.356 36.476 28.279 1.00 28.67
ATOM	717 CG1 ILE 248	49.555 36.571 26.543 1.00 28.83
ATOM	718 CD1 ILE 248	48.514 37.236 27.420 1.00 30.76
ATOM	719 C ILE 248	52.618 34.259 27.006 1.00 28.39
ATOM	720 O ILE 248	53.759 34.715 26.869 1.00 27.88
ATOM	721 N ILE 249	52.356 33.177 27.732 1.00 26.07
ATOM	722 CA ILE 249	53.413 32.474 28.454 1.00 27.37
ATOM	723 CB ILE 249	52.839 31.294 29.281 1.00 30.32
ATOM	724 CG2 ILE 249	53.958 30.425 29.840 1.00 31.29
ATOM	725 CG1 ILE 249	51.987 31.831 30.429 1.00 30.31
ATOM	726 CD1 ILE 249	51.295 30.753 31.230 1.00 31.30
ATOM	727 C ILE 249	54.510 31.974 27.509 1.00 28.63
ATOM	728 O ILE 249	55.701 32.100 27.808 1.00 29.59
ATOM	729 N LEU 250	54.110 31.442 26.357 1.00 29.03
ATOM	730 CA LEU 250	55.068 30.934 25.380 1.00 22.44
ATOM	731 CB LEU 250	54.351 30.166 24.266 1.00 24.30
ATOM	732 CG LEU 250	53.665 28.866 24.687 1.00 23.20
ATOM	733 CD1 LEU 250	52.951 28.273 23.502 1.00 20.36
ATOM	734 CD2 LEU 250	54.685 27.880 25.238 1.00 19.45
ATOM	735 C LEU 250	55.919 32.055 24.794 1.00 18.97
ATOM	736 O LEU 250	57.133 31.903 24.648 1.00 18.37
ATOM	737 N LEU 251	55.291 33.180 24.468 1.00 20.63
ATOM	738 CA LEU 251	56.026 34.318 23.915 1.00 27.43
ATOM	739 CB LEU 251	55.065 35.412 23.449 1.00 22.92
ATOM	740 CG LEU 251	54.364 35.093 22.128 1.00 24.72
ATOM	741 CD1 LEU 251	53.342 36.167 21.821 1.00 32.13
ATOM	742 CD2 LEU 251	55.389 34.981 21.009 1.00 22.46
ATOM	743 C LEU 251	57.026 34.875 24.930 1.00 27.23
ATOM	744 O LEU 251	58.202 35.078 24.614 1.00 26.48
ATOM	745 N LYS 252	56.561 35.094 26.156 1.00 27.34
ATOM	746 CA LYS 252	57.425 35.598 27.215 1.00 28.95
ATOM		56.649 35.715 28.527 1.00 32.89
ATOM		55.570 36.783 28.530 1.00 35.06
ATOM	749 CD LYS 252	55.084 37.028 29.943 1.00 42.82
ATOM	750 CE LYS 252	54.124 38.191 30.003 1.00 53.05
ATOM	751 NZ LYS 252	53.677 38.451 31.398 1.00 64.03
ATOM	752 C LYS 252	58.605 34.647 27.405 1.00 27.66
ATOM	753 O LYS 252	59.734 35.076 27.646 1.00 33.16
ATOM	754 N GLY 253	58.344 33.357 27.243 1.00 24.50
ATOM		59.386 32.364 27.402 1.00 22.33
ATOM	756 C GLY 253	60.423 32.273 26.297 1.00 23.99

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ATOM	757 O GLY 253	61.589 32.016 26.581 1.00 30.77
ATOM	758 N CYS 254	60.041 32.526 25.049 1.00 22.66
ATOM	759 CA CYS 254	60.986 32.405 23.934 1.00 20.75
ATOM	760 CB CYS 254	60.386 31.494 22.868 1.00 24.86
ATOM	761 SG CYS 254	58.996 32.276 22.014 1.00 25.55
ATOM	762 C CYS 254	61.399 33.702 23.242 1.00 23.79
ATOM	763 O CYS 254	62.262 33.685 22.357 1.00 22.18
ATOM	764 N CYS 255	60.788 34.814 23.625 1.00 19.49
ATOM	765 CA CYS 255	61.084 36.085 22.981 1.00 21.08
ATOM	766 CB CYS 255	60.336 37.220 23.669 1.00 18.21
ATOM	767 SG CYS 255	60.264 38.713 22.677 1.00 22.96
ATOM	768 C CYS 255	62.570 36.413 22.842 1.00 21.87
ATOM	769 O CYS 255	63.050 36.641 21.729 1.00 22.23
ATOM	770 N MET 256	63.310 36.397 23.947 1.00 20.82
ATOM	771 CA MET 256	64.741 36.706 23.895 1.00 20.50
ATOM	772 CB MET 256	65.322 36.801 25.312 1.00 22.50
ATOM	773 CG MET 256	66.808 37.139 25.354 1.00 16.67
ATOM	774 SD MET 256	67.205 38.732 24.605 1.00 24.46
ATOM	775 CE MET 256	69.027 38.764 24.791 1.00 19.21
ATOM	776 C MET 256	65.510 35.667 23.072 1.00 18.38
ATOM	777 O MET 256	66.401 36.005 22.293 1.00 17.68
ATOM	778 N GLU 257	65.149 34.404 23.248 1.00 20.33
ATOM	779 CA GLU 257	65.779 33.308 22.526 1.00 21.08
ATOM ATOM	780 CB GLU 257 781 CG GLU 257	65.148 31.982 22.943 1.00 22.28
ATOM	781 CG GLU 257 782 CD GLU 257	.65.374 31.640 24.411 1.00 34.68
ATOM	782 CD GLU 257	64.515 30.486 24.907 1.00 43.20 63.823 29.836 24.091 1.00 42.14
ATOM	784 OE2 GLU 257	63.823 29.836 24.091 1.00 42.14 64.530 30.230 26.128 1.00 50.15
ATOM	785 C GLU 257	65.650 33.503 21.018 1.00 19.26
ATOM	786 O GLU 257	66.632 33.360 20.276 1.00 18.09
ATOM	787 N ILE 258	64.446 33.850 20.566 1.00 16.30
ATOM	788 CA ILE 258	64.199 34.065 19.141 1.00 18.09
ATOM	789 CB ILE 258	62.677 34.150 18.825 1.00 18.61
ATOM	790 CG2 ILE 258	62.441 34.653 17.395 1.00 16.23
ATOM	791 CG1 ILE 258	62.032 32.771 19.021 1.00 13.80
ATOM	792 CD1 ILE 258	60.544 32.714 18.695 1.00 13.21
ATOM	793 C ILE 258	64.948 35.297 18.638 1.00 20.12
ATOM	794 O ILE 258	65.605 35.242 17.593 1.00 19.17
ATOM	795 N MET 259	64.903 36.387 19.404 1.00 22.71
ATOM	796 CA MET 259	65.602 37.611 19.015 1.00 17.09
ATOM	797 CB MET 259	65.249 38.772 19.941 1.00 18.80
ATOM	798 CG MET 259	63.782 39.159 19.894 1.00 17.66
ATOM	799 SD MET 259	63.457 40.748 20.678 1.00 25.77
ATOM	800 CE MET 259	63.774 40.377 22.374 1.00 16.65
ATOM	801 C MET 259	67.111 37.397 18.973 1.00 19.51
ATOM	802 O MET 259	67.797 37.913 18.080 1.00 25.53
ATOM	803 N SER 260	67.625 36.605 19.908 1.00 19.58

ATOM 804 CA SER 260 69.056 36.324 19.947 1.00 16.90 **ATOM** 805 CB SER 260 69.434 35.631 21.251 1.00 15.56 **ATOM** 806 OG SER 260 69.093 36.455 22.352 1.00 22.98 **ATOM** 807 C SER 260 69.471 35.487 18.746 1.00 14.52 **ATOM** 808 O SER 70.496 35.761 18.129 1.00 22.82 260 **ATOM** 809 N- LEU 261 68.663 34.490 18.397 1.00 16.50 **ATOM** 810 CA LEU 261 68.948 33.642 17.241 1.00 17.78 **ATOM** 811 CB LEU 261 67.878 32.552 17.092 1.00 18.38 **ATOM** 812 CG LEU 261 67.890 31.708 15.812 1.00 14.47 **ATOM** 813 CD1 LEU 261 69.159 30.877 15.728 1.00 16.76 **ATOM** 814 CD2 LEU 261 66.672 30.806 15.793 1.00 14.06 **ATOM** 815 C LEU 261 68.959 34.519 15.992 1.00 20.40 **ATOM** LEU 816 O 261 69.885 34.450 15.181 1.00 22.00 **ATOM** 817 N ARG 262 67.934 35.356 15.854 1.00 21.02 **ATOM** 818 CA ARG 262 67.821 36.249 14.705 1.00 22.84 **ATOM** 819 CB ARG 262 66.530 37.067 14.782 1.00 20.29 **ATOM** 820 CG ARG 262 65.311 36.267 14.364 1.00 23.33 ATOM 821 CD ARG 262 64.007 37.026 14.509 1.00 19.05 **ATOM** 822 NE ARG 262 62.959 36.321 13.775 1.00 21.32 **ATOM** 823 CZ ARG 262 61.780 36.837 13.441 1.00 23.44 **ATOM** 824 NH1 ARG 262 61.465 38.081 13.780 1.00 22.99 **ATOM** 825 NH2 ARG 262 60.933 36.116 12.713 1.00 22.09 **ATOM** 826 C ARG 262 69.035 37.154 14.561 1.00 22.66 **ATOM** 827 O ARG 262 69.434 37.483 13.445 1.00 22.41 **ATOM** 828 N ALA 263 69.625 37.545 15.689 1.00 23.52 **ATOM** 829 CA ALA 263 70.820 38.386 15.677 1.00 22.37 **ATOM** 830 CB ALA 263 70.986 39.089 17.018 1.00 22.76 **ATOM** 831 C ALA 263 72.052 37.530 15.366 1.00 22.85 **ATOM** 832 O ALA 263 72.882 37.897 14.529 1.00 25.50 **ATOM** 833 N ALA 264 72.131 36.365 16.005 1.00 21.68 **ATOM** 834 CA ALA 264 73.242 35.438 15.826 1.00 20.26 835 CB ALA 264 **ATOM** 73.092 34.256 16.763 1.00 15.97 **ATOM** 836 C ALA 264 73.401 34.957 14.382 1.00 23.11 **ATOM** 837 O ALA 264 74.523 34.831 13.892 1.00 24.87 **ATOM** 838 N VAL 265 72.293 34.679 13.697 1.00 22.94 **ATOM** 839 CA VAL 265 72.380 34.226 12.306 1.00 28.98 **ATOM** 840 CB VAL 265 71.072 33.547 11.797 1.00 25.97 **ATOM** 841 CG1 VAL 265 70.751 32.330 12.638 1.00 26.27 **ATOM** 842 CG2 VAL 265 69.907 34.527 11.797 1.00 26.64 **ATOM** 265 843 C VAL 72.761 35.373 11.369 1.00 28.81 **ATOM** 844 O VAL 72.966 35.160 10.176 1.00 31.92 265 **ATOM** 845 N ARG 72.830 36.587 11.915 1.00 31.83 266 **ATOM** 846 CA ARG 266 73.210 37.774 11.150 1.00 33.19 847 CB ARG **ATOM** 266 72.141 38.861 11.258 1.00 31.67 **ATOM** 848 CG ARG 266 70.986 38.623 10.320 1.00 26.82 **ATOM** 849 CD ARG 266 69.913 39.668 10.454 1.00 33.95 **ATOM** 850 NE ARG 266 68.955 39.532 9.361 1.00 38.15

ATOM -851 CZ ARG 67.688 39.927 9.410 1.00 37.39 266 **ATOM** 852 NH1 ARG 266 67.198 40.491 10.509 1.00 29.92 **ATOM** 853 NH2 ARG 266 66.918 39.770 8.340 1.00 31.24 **ATOM** 854 C ARG 266 74.565 38.307 11.604 1.00 36.31 **ATOM** 855 O ARG 266 74.821 39.516 11.575 1.00 38.56 **ATOM** 856 N- TYR 267 75.416 37.393 12.056 1.00 34.21 **ATOM** 857 CA TYR 267 76.755 37.733 12.502 1.00 35.24 **ATOM** 858 CB TYR 267 77.283 36.640 13.440 1.00 32.37 **ATOM** 859 CG TYR 267 78.774 36.699 13.703 1.00 35.07 **ATOM** 860 CD1 TYR 267 79.303 37.555 14.669 1.00 33.94 **ATOM** 861 CE1 TYR 267 80.677 37.609 14.905 1.00 36.60 **ATOM** 267 862 CD2 TYR 79.658 35.894 12.979 1.00 34.68 **ATOM** 863 CE2 TYR 81.029 35.940 13.208 1.00 36.07 267 **ATOM** 864 CZ TYR 267 81.533 36.797 14.170 1.00 37.14 **ATOM** 865 OH TYR 267 82.889 36.835 14.396 1.00 41.52 **ATOM** 866 C TYR 267 77.639 37.831 11.263 1.00 37.68 **ATOM** 867 O **TYR** 267 77.609 36.943 10.410 1.00 36.48 **ATOM** 868 N **ASP** 268 78.400 38.915 11.150 1.00 39.58 **ATOM** 869 CA ASP 268 79.301 39.096 10.016 1.00 42.77 **ATOM** 870 CB ASP 268 79.170 40.511 9.434 1.00 44.38 **ATOM** 871 CG ASP 268 80.145 40.770 8.290 1.00 50.31 **ATOM** 872 OD1 ASP 268 80.290 39.901 7.400 1.00 55.79 **ATOM** 873 OD2 ASP 268 80.773 41.847 8.280 1.00 50.24 **ATOM** 874 C ASP 268 80.737 38.846 10.466 1.00 42.51 **ATOM ASP** 875 O 268 81.305 39.645 11.208 1.00 42.75 269 **ATOM** 876 N PRO 81.346 37.733 10.020 1.00 44.56 **ATOM** 877 CD PRO 269 80.770 36.697 9.146 1.00 42.66 **ATOM** 878 CA PRO 269 82.725 37.395 10.393 1.00 45.98 879 CB PRO **ATOM** 269 82.991 36.111 9.607 1.00 44.04 **ATOM** 880 CG PRO 269 81.631 35.506 9.458 1.00 43.33 **ATOM** 881 C PRO 269 83.710 38.492 10.004 1.00 50.31 **ATOM** 882 O **PRO** 269 84.630 38.800 10.761 1.00 49.83 270 **ATOM** 883 N ALA 83.486 39.100 8.840 1.00 53.62 **ATOM** 884 CA ALA 270 84.348 40.165 8.329 1.00 54.54 **ATOM** 885 CB ALA 270 83.892 40.585 6.929 1.00 51.24 **ATOM** 886 C ALA 270 9.248 1.00 55.69 84.449 41.389 **ATOM** 887 O ALA 270 85.488 42.045 9.294 1.00 57.92 **ATOM** 888 N SER 271 83.384 41.685 9.989 1.00 54.71 **ATOM** 889 CA SER 271 83.378 42.838 10.889 1.00 51.26 **ATOM** 890 CB SER 271 82.182 43.740 10.575 1.00 49.92 82.065 43.976 9.183 1.00 60.09 **ATOM** 891 OG SER 271 **ATOM** 892 C SER 271 83.305 42.443 12.360 1.00 50.78 **ATOM** 893 O SER 271 83.482 43.288 13.240 1.00 52.11 **ATOM** 894 N **ASP** 272 83.051 41.162 12.619 1.00 48.96 272 **ATOM** 895 CA ASP 82.898 40.643 13.978 1.00 45.53 84.206 40.765 14.776 1.00 44.82 **ATOM** 896 CB ASP 272 84.142 40.064 16.131 1.00 47.66 **ATOM** 897 CG ASP 272

ATOM 898 OD1 ASP 84.750 40.581 17.091 1.00 48.64 272 **ATOM** 899 OD2 ASP 272 83.495 38.999 16.238 1.00 43.85 **ATOM** 900 C **ASP** 272 81.765 41.437 14.636 1.00 44.46 **ATOM** 901 O **ASP** 272 81.904 41.958 15.747 1.00 42.41 902 N ATOM THR 273 80.652 41.551 13.915 1.00 39.79 **ATOM** 903 CA THR 273 79.492 42.282 14.401 1.00 38.82 **ATOM** 273 904 CB THR 79.334 43.648 13.670 1.00 39.73 **ATOM** 905 OG1 THR 273 79.288 43.439 12.254 1.00 39.36 **ATOM** 906 CG2 THR 273 80.496 44.578 13.991 1.00 41.31 **ATOM** 907 C THR 273 78.203 41.485 14.211 1.00 38.36 **ATOM** 908 O THR 273 78.151 40.546 13.408 1.00 33.79 **ATOM** 909 N LEU 274 77.187 41.835 14.995 1.00 36.91 **ATOM** 910 CA LEU 274 75.869 41.212 14.912 1.00 34.49 ATOM 911 CB LEU 274 75.342 40.822 16.297 1.00 30.37 **ATOM** 912 CG LEU 274 75.948 39.651 17.069 1.00 32.97 **ATOM** 913 CD1 LEU 274 75.297 39.593 18.440 1.00 28.23 **ATOM** 914 CD2 LEU 274 75.749 38.341 16.318 1.00 26.86 **ATOM** 915 C 74.956 42.289 14.352 1.00 35.35 LEU 274 **ATOM** 916 O LEU 274 75.171 43.478 14.601 1.00 37.47 **ATOM** 917 N THR 275 73.942 41.890 13.599 1.00 34.05 **ATOM** 918 CA THR 275 73.020 42.868 13.052 1.00 32.62 **ATOM** 919 CB THR 275 72.824 42.674 11.542 1.00 35.14 **ATOM** 920 OG1 THR 275 74.108 42.590 10.909 1.00 39.50 **ATOM** 921 CG2 THR 275 72.064 43.851 10.952 1.00 30.94 **ATOM** 922 C THR 275 71.699 42.746 13.793 1.00 30.92 **ATOM** 923 O THR 275 71.100 41.670 13.845 1.00 36.53 924 N LEU 276 **ATOM** 71.291 43.835 14.434 1.00 28.10 **ATOM** 925 CA LEU 276 70.051 43.868 15.192 1.00 27.78 **ATOM 926 CB LEU** 276 70.205 44.780 16.420 1.00 22.51 **ATOM** 927 CG LEU 276 71.383 44.532 17.373 1.00 25.89 **ATOM** 928 CD1 LEU 276 71.225 45.408 18.608 1.00 20.70 **ATOM** 929 CD2 LEU 276 71.456 43.069 17.782 1.00 20.79 **ATOM** 930 C LEU 276 68.930 44.376 14.296 1.00 27.27 **ATOM** 931 O LEU 276 69.068 45.430 13.672 1.00 29.06 **ATOM** 932 N SER 277 67.854 43.598 14:187 1.00 25.97 **ATOM** 933 CA SER 277 66.697 43.957 13.366 1.00 28.63 **ATOM** 934 CB SER 277 65.990 45.177 13.967 1.00 27.78 **ATOM** 935 OG SER 277 65.561 44.905 15.290 1.00 22.65 **ATOM** 936 C SER 277 67.067 44.209 11.897 1.00 30.31 **ATOM** 937 O SER 277 66.374 44.939 11.181 1.00 28.52 278 **ATOM** 938 N GLY 68.168 43.597 11.465 1.00 31.24 **ATOM** 939 CA GLY 68.638 43.754 10.101 1.00 39.59 278 **ATOM** 940 C GLY 278 68.999 45.178 9.706 1.00 44.55 **ATOM** 941 O **GLY** 278 69.104 45.479 8.517 1.00 46.66 **ATOM** 942 N GLU 279 69.234 46.046 10.686 1.00 43.47 **ATOM** 943 CA GLU 279 69.566 47.435 10.387 1.00 43.87 **ATOM** 944 CB GLU 279 68.314 48.312 10.515 1.00 44.28

ATOM	945 CG GLU 279	67.703 48.322 11.908 1.00 52.30
ATOM	· · ·	66.440 49.159 12.001 1.00 60.23
ATOM		66.398 50.074 12.853 1.00 63.06
ATOM	948 OE2 GLU 279	65.485 48.894 11.238 1.00 65.67
ATOM	949 C GLU 279	70.700 48.038 11.216 1.00 42.40
ATOM	950 O GLU 279	71.330 49.001 10.787 1.00 43.89
ATOM	951 N MET 280	70.977 47.472 12.388 1.00 40.86
ATOM	952 CA MET 280	72.027 48.009 13.248 1.00 32.80
ATOM	953 CB MET 280	71.435 48.415 14.603 1.00 29.25
ATOM	954 CG MET 280	72.384 49.193 15.506 1.00 31.64
ATOM	955 SD MET 280	71.830 49.235 17.232 1.00 34.02
ATOM	956 CE MET 280	70.566 50.495 17.197 1.00 26.56
ATOM	957 C MET 280	73.172 47.033 13.465 1.00 32.77
ATOM	958 O MET 280	72.983 45.971 14.058 1.00 34.61
ATOM	959 N ALA 281	74.351 47.375 12.959 1.00 31.87
ATOM	960 CA ALA 281	75.523 46.526 13.147 1.00 34.71
ATOM	961 CB ALA 281	76.519 46.727 12.023 1.00 34.42
ATOM	962 C ALA 281	76.125 46.950 14.482 1.00 36.76
ATOM	963 O ALA 281	76.416 48.129 14.693 1.00 34.59
ATOM	964 N VAL 282	76.275 45.993 15.390 1.00 37.16
ATOM	965 CA VAL 282	76.798 46.263 16.721 1.00 37.83
ATOM	966 CB VAL 282	75.692 46.023 17.780 1.00 37.58
ATOM	967 CG1 VAL 282	76.219 46.271 19.175 1.00 48.99
ATOM	968 CG2 VAL 282	74.514 46.939 17.514 1.00 43.59
ATOM	969 C VAL 282	78.017 45.400 17.046 1.00 39.04
ATOM	970 O VAL 282	78.081 44.230 16.660 1.00 39.16
ATOM	971 N LYS 283	78.989 45.993 17.735 1.00 38.75
ATOM	972 CA LYS 283	80.205 45.287 18.136 1.00 42.18
ATOM	973 CB LYS 283	81.428 46.208 18.045 1.00 47.46
ATOM	974 CG LYS 283	81.803 46.617 16.632 1.00 51.71
ATOM	975 CD LYS 283	83.092 47.416 16.618 1.00 59.26
ATOM	976 CE LYS 283	83.481 47.813 15.202 1.00 62.52
ATOM	977 NZ LYS 283	82.492 48.742 14.588 1.00 66.27
ATOM	978 C LYS 283	80.075 44.746 19.559 1.00 38.78
ATOM	979 O LYS 283	79.283 45.257 20:356 1.00 40.63
ATOM	980 N ARG 284	80.900 43.753 19.881 1.00 36.01
ATOM	981 CA ARG 284	80.908 43.104 21.189 1.00 38.62
ATOM	982 CB ARG 284	82.150 42.224 21.327 1.00 38.83
ATOM	983 CG ARG 284	82.220 41.091 20.333 1.00 41.87
ATOM	984 CD ARG 284	83.521 40.335 20.451 1.00 39.60
ATOM	985 NE ARG 284	83.506 39.120 19.644 1.00 45.18
ATOM	986 CZ ARG 284	83.259 37.905 20.128 1.00 44.79
ATOM	987 NH1 ARG 284	83.005 37.739 21.421 1.00 41.84
ATOM	988 NH2 ARG 284	83.271 36.852 19.319 1.00 42.27
ATOM	989 C ARG 284	80.829 44.051 22.385 1.00 41.18
ATOM	990 O ARG 284	79.995 43.867 23.274 1.00 44.38
ATOM	991 N GLU 285	81.703 45.052 22.416 1.00 38.71

ATOM	1 992 CA GLU 285	81.724 46.002 23.525 1.00 37.18
ATOM	f 993 CB GLU 285	82.950 46.906 23.422 1.00 36.65
ATOM	1 994 C GLU 285	80.444 46.838 23.614 1.00 35.71
ATOM	I 995 O GLU 285	79.921 47.074 24.704 1.00 33.00
ATOM	I 996 N GLN 286	79.920 47.245 22.463 1.00 32.01
ATOM	_	78.714 48.061 22.425 1.00 32.31
ATOM		78.440 48.525 20.997 1.00 38.24
ATOM		79.565 49.352 20.392 1.00 42.42
ATOM		79.277 49.761 18.964 1.00 44.79
ATOM		79.103 48.910 18.089 1.00 42.21
ATOM		79.215 51.063 18.719 1.00 47.53
ATOM		77.484 47.355 23.002 1.00 33.08
ATOM		76.770 47.929 23.827 1.00 30.95
ATOM		77.245 46.114 22.579 1.00 31.49
ATOM		76.095 45.350 23.068 1.00 31.01
ATOM		75.892 44.073 22.242 1.00 24.63
ATOM	·	74.498 43.780 21.661 1.00 27.34
ATOM		74.382 42.282 21.359 1.00 20.50
ATOM		73.393 44.205 22.616 1.00 14.41
ATOM	1011 C LEU 287	76.298 44.986 24.538 1.00 32.80
ATOM	1012 O LEU 287	75.351 45.014 25.334 1.00 32.10
ATOM		77.536 44.641 24.885 1.00 32.54
ATOM	1014 CA LYS 288	77.897 44.280 26.251 1.00 30.70
ATOM	1015 CB LYS 288	79.376 43.893 26.315 1.00 31.24
ATOM	1016 CG LYS 288	79.834 43.382 27.662 1.00 34.69
ATOM	1017 CD LYS 288	81.227 42.784 27.574 1.00 37.69
ATOM	1018 CE LYS 288	81.638 42.177 28.904 1.00 42.86
ATOM	1019 NZ LYS 288	82.883 41.369 28.786 1.00 49.63
ATOM	1020 C LYS 288	77.611 45.448 27.189 1.00 28.74
ATOM	1021 O LYS 288	76.827 45.319 28.129 1.00 34.45
ATOM	1022 N ASN 289	78.190 46.602 26.882 1.00 26.57
ATOM	1023 CA ASN 289	78.011 47.803 27.691 1.00 30.84
ATOM	1024 CB ASN 289	79.012 48.879 27.274 1.00 26.04
ATOM	1025 CG ASN 289	80.437 48.485 27.570 1.00 35.16
ATOM	1026 OD1 ASN 289	80.700 47.718 28.499 1.00 42.54
ATOM	1027 ND2 ASN 289	81.371 48.998 26.784 1.00 32.82
ATOM	1028 C ASN 289	76.602 48.371 27.620 1.00 35.05
ATOM	1029 O ASN 289	76.154 49.039 28.550 1.00 36.94
ATOM	1030 N GLY 290	75.909 48.113 26.515 1.00 32.43
ATOM	1031 CA GLY 290	74.556 48.614 26.345 1.00 28.66
ATOM	1032 C GLY 290	73.525 48.024 27.289 1.00 28.48
ATOM	1033 O GLY 290	72.377 48.467 27.308 1.00 28.17
ATOM	1034 N GLY 291	73.908 47.002 28.047 1.00 28.66
ATOM	1035 CA GLY 291	72.969 46.408 28.980 1.00 29.19
ATOM	1036 C GLY 291	72.976 44.894 29.075 1.00 29.76
ATOM	1037 O GLY 291	72.595 44.340 30.105 1.00 34.44
ATOM	1038 N LEU 292	73.399 44.213 28.017 1.00 29.69
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ATOM 1039 CA LEU 292 73.410 42.755 28.036 1.00 30.64 **ATOM** 1040 CB LEU 292 73.421 42.194 26.611 1.00 27.07 ATOM 1041 CG LEU 292 72.113 42.348 25.833 1.00 23,27 **ATOM** 1042 CD1 LEU 292 72.202 41.580 24.532 1.00 22.24 **ATOM** 1043 CD2 LEU 292 70.950 41.827 26.661 1.00 23.80 **ATOM** 1044 C LEU 292 74.530 42.125 28.861 1.00 29.22 **ATOM** 1045 O LEU 292 74.365 41.033 29.404 1.00 31.02 **ATOM** 1046 N **GLY** 293 75.671 42.800 28.945 1.00 30,26 **ATOM** 1047 CA GLY 293 76.788 42.259 29.700 1.00 28.37 **ATOM** 1048 C **GLY** 293 77.307 40.995 29.040 1.00 29.85 **ATOM** 1049 O GLY 77.460 40.951 27.820 1.00 32.37 293 **ATOM** 1050 N VAL 294 77.537 39.953 29.832 1.00 30.08 **ATOM** 1051 CA VAL 294 78.041 38.687 29.308 1.00 31.62 **ATOM** 1052 CB VAL 294 78.466 37.716 30.442 1.00 29.11 **ATOM** 1053 CG1 VAL 294 79.649 38.292 31.191 1.00 31.37 1054 CG2 VAL **ATOM** 294 77.304 37.443 31.396 1.00 26.69 ATOM 1055 C VAL 294 77.079 37.978 28.351 1.00 32.81 **ATOM** 1056 O VAL 294 77.496 37.095 27.591 1.00 33.00 **ATOM** 1057 N VAL 295 75.801 38.356 28.380 1.00 30.45 **ATOM** 1058 CA VAL 295 74.814 37.752 27.487 1.00 28.02 **ATOM** 1059 CB VAL 295 73.378 38.232 27.793 1.00 29.96 **ATOM** 295 1060 CG1 VAL 72.380 37.575 26.838 1.00 22.55 **ATOM** 1061 CG2 VAL 295 73.016 37.903 29.232 1.00 20.10 ATOM 1062 C VAL 295 75.203 38.115 26.057 1.00 29.90 **ATOM** 1063 O VAL 295 75.047 37.312 25.140 1.00 34.47 **ATOM** 1064 N SER 296 75.762 39.309 25.886 1.00 29.11 1065 CA SER **ATOM** 296 76.215 39.771 24.581 1.00 30.96 **ATOM** 1066 CB SER 296 76.785 41.184 24.702 1.00 27.26 **ATOM** 296 1067 OG SER 77.300 41.648 23.469 1.00 22.93 **ATOM** 1068 C SER 296 77.294 38.811 24.080 1.00 36.41 **ATOM SER** 1069 O 296 77.238 38.341 22.939 1.00 38.84 **ATOM** 1070 N **ASP** 297 78.254 38.501 24.954 1.00 35.29 **ATOM** 1071 CA ASP 297 79.346 37.585 24.629 1.00 32.14 **ATOM** 1072 CB ASP 297 80.245 37.356 25.851 1.00 36.57 1073 CG ASP 297 **ATOM** 80.958 38.616 26.307 1.00 41.75 **ATOM** 1074 OD1 ASP 297 81.492 39.352 25.447 1.00 45.45 **ATOM** 1075 OD2 ASP 297 80.999 38.861 27.532 1.00 45.15 1076 C **ATOM ASP** 297 78.768 36.249 24.191 1.00 29.61 **ATOM** 1077 O **ASP** 297 79.242 35.644 23.231 1.00 32.90 **ATOM** 1078 N ALA 298 77.738 35.804 24.903 1.00 27.85 **ATOM** 1079 CA ALA 298 77.071 34.544 24.608 1.00 27.89 **ATOM** 1080 CB ALA 298 75.998 34.258 25.657 1.00 21.67 ALA **ATOM** 1081 C 298 76.462 34.539 23.202 1.00 28.26 ALA 298 **ATOM** 1082 O 76.648 33.579 22.446 1.00 30.19 **ATOM** 1083 N ILE 299 75.744 35.606 22.853 1.00 25.20 **ATOM** 1084 CA ILE 299 75.119 35.708 21.537 1.00 23.46 **ATOM** 1085 CB ILE 299 74.200 36.944 21.427 1.00 21.63

ATOM 1086 CG2 ILE 299 73.491 36.946 20.078 1.00 22.20 **ATOM** 1087 CG1 ILE 299 73.145 36.914 22.536 1.00 19.79 **ATOM** 1088 CD1 ILE 299 72.245 38.139 22.578 1.00 18.33 **ATOM** 1089 C ILE 299 76.181 35.752 20.444 1.00 26.28 **ATOM** 1090 O ILE 299 76.043 35.095 19.414 1.00 31.72 **ATOM** 1091 N- PHE 300 77.247 36.512 20.675 1.00 29.35 **ATOM** 1092 CA PHE 300 78.338 36.613 19.709 1.00 29.01 **ATOM** 300 1093 CB PHE 79.386 37.622 20.182 1.00 29.53 **ATOM** 1094 CG PHE 300 79.239 38.978 19.562 1.00 27.60 **ATOM** 1095 CD1 PHE 300 78.481 39.964 20.179 1.00 24.86 **ATOM** 1096 CD2 PHE 300 79.853 39.266 18.350 1.00 27.39 78.337 41.218 19.597 1.00 25.66 ATOM 1097 CE1 PHE 300 **ATOM** 1098 CE2 PHE 300 79.715 40.518 17.761 1.00 25.97 **ATOM** 1099 CZ PHE 300 78.956 41.495 18.384 1.00 21.03 ATOM 1100 C PHE 300 78.988 35.248 19.496 1.00 30.34 1101 O PHE 300 **ATOM** 79.309 34.873 18.367 1.00 29.35 ATOM 1102 N GLU 301 79.181 34.507 20.582 1.00 31.04 **ATOM** 1103 CA GLU 301 79.775 33.178 20.499 1.00 33.60 **ATOM** 1104 CB GLU 301 80.012 32.607 21.898 1.00 31.64 **ATOM** 1105 C **GLU** 78.851 32.265 19.696 1.00 33.90 301 **ATOM** 1106 O **GLU** 301 79.315 31.473 18.872 1.00 33.33 **ATOM** 1107 N LEU 302 77.546 32.386 19.935 1.00 31.13 ATOM 1108 CA LEU 302 76.556 31.581 19.227 1.00 27.57 **ATOM** 1109 CB LEU 302 75.150 31.842 19.776 1.00 25.24 **ATOM** 1110 CG LEU 302 73.994 31.131 19.059 1.00 28.59 **ATOM** 1111 CD1 LEU 302 74.066 29.634 19.299 1.00 25.52 **ATOM** 1112 CD2 LEU 302 72.660 31.682 19.532 1.00 19.30 **ATOM** 1113 C LEU 302 76.601 31.904 17.739 1.00 26.80 **ATOM** 1114 O LEU 302 76.682 31.003 16.904 1.00 27.81 **ATOM** 1115 N **GLY** 303 76.576 33.195 17.416 1.00 26.47 **ATOM** 1116 CA GLY 303 76.611 33.624 16.030 1.00 26.99 **GLY** ATOM 1117 C 303 77.845 33.133 15.295 1.00 33.46 **ATOM** 1118 O **GLY** 303 77.757 32.646 14.164 1.00 32.33 **ATOM** 1119 N LYS 304 78.994 33.232 15.956 1.00 34.63 304 80.269 32.813 15.383 1.00 36.20 **ATOM** 1120 CA LYS 1121 CB LYS 304 ATOM 81.399 33.115 16.372 1.00 41.96 **ATOM** 1122 CG LYS 304 82.779 33.179 15.757 1.00 47.05 **ATOM** 1123 CD LYS 304 83.800 33.610 16.796 1.00 59.47 **ATOM** 1124 CE LYS 304 85.179 33.791 16.181 1.00 65.89 **ATOM** 1125 NZ LYS 304 85.182 34.863 15.144 1.00 71.01 ATOM 1126 C LYS 304 80.276 31.332 14.992 1.00 33.17 **ATOM** 1127 O LYS 304 80.752 30.974 13.913 1.00 34.44 **ATOM** 1128 N SER 305 79.739 30.482 15.861 1.00 31.40. **ATOM** 1129 CA SER 305 79.687 29.048 15.594 1.00 33.10 79.513 28.266 16.900 1.00 34.10 **ATOM** 1130 CB SER 305 **ATOM** 305 1131 OG SER 78.391 28.727 17.633 1.00 40.61 **ATOM** 1132 C SER 305 78.597 28.664 14.589 1.00 33.02

ATOM	1133 O SER 305	78.771 27.718 13.816 1.00 35.32
ATOM	1134 N LEU 306	77.488 29.404 14.580 1.00 32.14
ATOM	1135 CA LEU 306	76.391 29.121 13.653 1.00 31.02
ATOM	1136 CB LEU 306	75.138 29.936 13.996 1.00 22.76
ATOM	1137 CG LEU 306	74.361 29.487 15.235 1.00 24.42
ATOM	1138 CD1 LEU 306	73.094 30.311 15.380 1.00 23.13
ATOM	1139 CD2 LEU 306	74.016 28.009 15.126 1.00 25.53
ATOM	1140 C LEU 306	76.780 29.354 12.198 1.00 33.11
ATOM	1141 O LEU 306	76.161 28.796 11.293 1.00 32.60
ATOM	1142 N SER 307	77.821 30.153 11.975 1.00 36.12
ATOM	1143 CA SER 307	78.296 30.448 10.624 1.00 38.80
ATOM	1144 CB SER 307	79.514 31.373 10.677 1.00 41.64
ATOM	1145 OG SER 307	79.224 32.556 11.401 1.00 54.66
ATOM	1146 C SER 307	78.650 29.182 9.845 1.00 36.98
ATOM	1147 O SER 307	78.302 29.055 8.669 1.00 42.87
ATOM	1148 N ALA 308	79.315 28.239 10.509 1.00 35.72
ATOM	1149 CA ALA 308	79.719 26.983 9.879 1.00 32.70
ATOM	1150 CB ALA 308	80.683 26.227 10.782 1.00 33.88
ATOM	1151 C ALA 308	78.531 26.093 9.521 1.00 34.83
ATOM	1152 O ALA 308	78.620 25.278 8.600 1.00 39.61
ATOM	1153 N PHE 309	77.424 26.250 10.244 1.00 31.54
ATOM	1154 CA PHE 309	76.226 25.453 9.999 1.00 32.43
ATOM	1155 CB PHE 309	75.259 25.558 11.182 1.00 30.89
ATOM	1156 CG PHE 309	75.718 24.826 12.415 1.00 33.73
ATOM	1157 CD1 PHE 309	76.769 25.314 13.183 1.00 40.48
ATOM	1158 CD2 PHE 309	75.091 23.654 12.816 1.00 35.96
ATOM	1159 CE1 PHE 309	77.189 24.643 14.334 1.00 37.87
ATOM	1160 CE2 PHE 309	75.502 22.975 13.962 1.00 38.44
ATOM	1161 CZ PHE 309	76.553 23.471 14.722 1.00 37.34
ATOM	1162 C PHE 309	75.507 25.809 8.693 1.00 34.76
ATOM	1163 O PHE 309	74.810 24.969 8.118 1.00 36.18
ATOM	1164 N ASN 310	75.693 27.040 8.218 1.00 35.80
	1165 CA ASN 310	75.060 27.506 6.980 1.00 41.00
ATOM	1166 CB ASN 310	75.705 26.852 5.755 1.00 51.94
ATOM	1167 CG ASN 310	77.053 27.452 5.419 1.00 67.92
ATOM	1168 OD1 ASN 310	77.139 28.439 4.687 1.00 77.32
ATOM	1169 ND2 ASN 310	78.116 26.869 5.962 1.00 72.62
ATOM		73.560 27.245 6.985 1.00 38.15
ATOM'	1171 O ASN 310	73.034 26.515 6.141 1.00 35.87
ATOM	1172 N LEU 311	72.885 27.819 7.971 1.00 33.94
ATOM	1173 CA LEU 311	71.450 27.651 8.111 1.00 32.09
ATOM	1174 CB LEU 311	71.011 28.009 9.533 1.00 28.06
ATOM	1175 CG LEU 311	71.656 27.301 10.724 1.00 26.38
ATOM	1176 CD1 LEU 311	71.092 27.883 12.012 1.00 23.56
ATOM	1177 CD2 LEU 311	71.409 25.801 10.651 1.00 21.24
ATOM	1178 C LEU 311	70.705 28.542 7.124 1.00 33.00
ATOM	1179 O LEU 311	71.173 29.630 6.782 1.00 35.47

ATOM	1180 N ASP 312	69.569 28.057 6.638 1.00 27.78
ATOM	1181 CA ASP 312	68.749 28.841 5.733 1.00 27.06
ATOM	1182 CB ASP 312	68.385 28.049 4.456 1.00 25.84
ATOM	1183 CG ASP 312	67.580 26.778 4.724 1.00 25.67
ATOM	1184 OD1 ASP 312	67.124 26.541 5.860 1.00 28.20
ATOM	1185 OD2 ASP 312	67.387 26.008 3.762 1.00 27.62
ATOM		67.517 29.314 6.514 1.00 28.51
ATOM	1187 O ASP 312	67.371 28.990 7.703 1.00 25.35
ATOM	1188 N ASP 313	66.633 30.060 5.855 1.00 22.16
ATOM	1189 CA ASP 313	65.430 30.589 6.494 1.00 21.37
ATOM	1190 CB ASP 313	64.625 31.431 5.499 1.00 25.11
ATOM	1191 CG ASP 313	65.380 32.666 5.025 1.00 31.54
ATOM	1192 OD1 ASP 313	65.119 33.115 3.890 1.00 35.35
ATOM	1193 OD2 ASP 313	66.225 33.193 5.783 1.00 35.37
ATOM	1194 C ASP 313	64.524 29.535 7.120 1.00 21.11
ATOM	1195 O ASP 313	63.904 29.783 8.158 1.00 23.68
ATOM	1196 N THR 314	64.440 28.367 6.489 1.00 22.88
ATOM	1197 CA THR 314	63.591 27.281 6.981 1.00 22.81
ATOM	1198 CB THR 314	63.472 26.155 5.927 1.00 26.00
ATOM	1199 OG1 THR 314	62.873 26.679 4.732 1.00 20.14
ATOM	1200 CG2 THR 314	62.629 25.010 6.457 1.00 17.51
ATOM	1201 C THR 314	64.086 26.706 8.310 1.00 19.46
ATOM	1202 O THR 314	63.312 26.529 9.247 1.00 19.33
ATOM	1203 N GLU 315	65.381 26.431 8.392 1.00 17.49
ATOM	1204 CA GLU 315	65.965 25.885 9.611 1.00 20.62
ATOM	1205 CB GLU 315	67.426 25.514 9.358 1.00 14.39
ATOM	1206 CG GLU 315	67.539 24.339 8.400 1.00 13.07
ATOM	1207 CD GLU 315	68.923 24.125 7.835 1.00 14.98
ATOM	1208 OE1 GLU 315	69.634 25.116 7.552 1.00 17.71
ATOM	1209 OE2 GLU 315	69.287 22.948 7.651 1.00 17.88
ATOM	1210 C GLU 315	65.810 26.883 10.762 1.00 20.57
ATOM	1211 O GLU 315	65.368 26.518 11.854 1.00 18.43
ATOM	1212 N VAL 316	66.096 28.154 10.488 1.00 19.19
ATOM	1213 CA VAL 316	65.955 29.203 11.490 1.00 16.53
ATOM	1214 CB VAL 316	66.418 30.567 10.933 1.00 17.42
ATOM	1215 CG1 VAL 316	66.149 31.687 11.940 1.00 13.89
ATOM	1216 CG2 VAL 316	67.900 30.506 10.594 1.00 14.31
ATOM	1217 C VAL 316	64.488 29.291 11.927 1.00 19.53
ATOM	1218 O VAL 316	64.191 29.448 13.110 1.00 19.86
ATOM	1219 N ALA 317	63.575 29.159 10.970 1.00 19.02
ATOM	1220 CA ALA 317	62.145 29.215 11.254 1.00 16.95
ATOM	1221 CB ALA 317	61.357 29.239 9.951 1.00 17.68
ATOM	1222 C ALA 317	61.674 28.047 12.126 1.00 14.13
ATOM	1223 O ALA 317	60.875 28.228 13.045 1.00 15.34
ATOM	1224 N LEU 318	62.154 26.847 11.819 1.00 17.41
ATOM	1225 CA LEU 318	61.769 25.653 12.569 1.00 19.10
ATOM	1226 CB LEU 318	62.186 24.398 11.802 1.00 18.21

ATOM 1227 CG LEU 318 61.443 24.209 10.473 1.00 19.02 **ATOM** 1228 CD1 LEU 318 62.105 23.128 9.646 1.00 16.10 **ATOM** 1229 CD2 LEU 318 59.987 23.875 10.735 1.00 11.32 1230 C **ATOM** LEU 318 62.399 25.685 13.954 1.00 22.38 **ATOM** 1231 O LEU 318 61.782 25.278 14.945 1.00 21.64 **ATOM** 1232 N- LEU 319 63.619 26.207 14.016 1.00 20.97 **ATOM** 1233 CA LEU 319 64.338 26.344 15.270 1.00 19.71 ATOM 1234 CB LEU 319 65.715 26.951 15.005 1.00 20.56 1235 CG LEU 319 ATOM 66.722 27.036 16.152 1.00 32.05 ATOM 1236 CD1 LEU 319 66.704 25.760 16.963 1.00 33.15 **ATOM** 1237 CD2 LEU 319 68.109 27.303 15.590 1.00 28.25 **ATOM** 1238 C LEU 319 63.496 27.254 16.164 1.00 20.66 ATOM 1239 O LEU 319 63.215 26.920 17.313 1.00 24.47 **ATOM** 1240 N GLN 320 63.026 28.365 15.604 1.00 19.25 **ATOM** 1241 CA GLN 320 62.191 29.307 16.346 1.00 19.02 **ATOM** 1242 CB GLN 320 61.842 30.526 15.488 1.00 19.11 **ATOM** 1243 CG GLN 320 63.032 31.377 15.101 1.00 20.02 **ATOM** 1244 CD GLN 320 62.665 32.562 14.224 1.00 23.65 **ATOM** 1245 OE1 GLN 320 63.487 33.445 13.997 1.00 22.68 **ATOM** 1246 NE2 GLN 320 61.440 32.574 13.704 1.00 20.77 **ATOM** 1247 C GLN 60.905 28.635 16.811 1.00 20.52 320 ATOM 1248 O GLN 320 60.465 28.845 17.938 1.00 22.04 **ATOM** 1249 N ALA 321 60.306 27.825 15.942 1.00 21.01 1250 CA ALA 321 59.069 27.128 16.280 1.00 16.83 ATOM ATOM 1251 CB ALA 321 58.556 26.358 15.079 1.00 16.58 **ATOM** 1252 C ALA 321 59.288 26.185 17.462 1.00 18.15 **ATOM** 1253 O ALA 321 58.427 26.069 18.344 1.00 13.03 **ATOM** 1254 N VAL 322 60.442 25.523 17.481 1.00 14.89 ATOM 1255 CA VAL 322 60.774 24.599 18.559 1.00 19.05 **ATOM** 1256 CB VAL 322 62.051 23.779 18.233 1.00 21.50 **ATOM** 1257 CG1 VAL 322 62.510 22.990 19.457 1.00 21.49 **ATOM** 1258 CG2 VAL 322 61.773 22.819 17.073 1.00 15.42 **ATOM** 1259 C VAL 322 60.947 25.375 19.867 1.00 19.89 VAL **ATOM** 1260 O 322 60.478 24.940 20.919 1.00 21.58 1261 N LEU **ATOM** 323 61.591 26.537 19.788 1.00 20.25 1262 CA LEU ATOM 323 61.804 27.387 20.959 1.00 19.32 1263 CB LEU 323 **ATOM** 62.683 28.586 20.597 1.00 12.95 1264 CG LEU 323 ATOM 64.129 28.273 20.217 1.00 20.70 1265 CD1 LEU 323 **ATOM** 64.805 29.503 19.641 1.00 13.23 **ATOM** 1266 CD2 LEU 323 64.883 27.767 21.438 1.00 22.91 **ATOM** 1267 C LEU 323 60.468 27.884 21.497 1.00 20.25 ATOM 1268 O LEU 323 60.251 27.918 22.706 1.00 25.88 **ATOM** 1269 N LEU 324 59.571 28.251 20.587 1.00 23.08 1270 CA LEU **ATOM** 324 58.248 28.753 20.944 1.00 21.24 1271 CB LEU **ATOM** 324 57.555 29.333 19.707 1.00 18.45 **ATOM** 1272 CG LEU 324 56.119 29.847 19.868 1.00 17.07 **ATOM** 1273 CD1 LEU 324 56.083 31.092 20.752 1.00 15.39

ATOM 1274 CD2 LEU 324 55.545 30.162 18.498 1.00 17.90 **ATOM** 1275 C LEU 324 57.342 27.706 21.598 1.00 21.54 **ATOM** 1276 O LEU 324 56.742 27.967 22.642 1.00 23.41 **ATOM** 1277 N **MET** 325 57.249 26.521 21.003 1.00 24.63 **ATOM** 1278 CA MET 325 56.380 25.476 21.545 1.00 25.35 **ATOM** 1279 CB MET 325 55.901 24.536 20.430 1.00 25.53 **ATOM** 1280 CG MET 325 55.235 25.220 19.232 1.00 21.89 **ATOM** 1281 SD MET 325 53.871 26.337 19.649 1.00 25.50 1282 CE MET **ATOM** 325 52.705 25.250 20.397 1.00 17.66 1283 C **ATOM MET** 325 57.031 24.676 22.675 1.00 27.58 **ATOM** 1284 O **MET** 325 56.988 23.450 22.690 1.00 28.61 ATOM 1285 N SER 326 57.613 25.376 23.638 1.00 27.98 **ATOM** 1286 CA SER 326 58.265 24.718 24.757 1.00 31.60 ATOM 1287 CB SER 326 59.527 25.493 25.155 1.00 35.80 **ATOM** 1288 OG SER 326 60.123 24.966 26.327 1.00 43.74 **ATOM** 1289 C SER 57.313 24.624 25.939 1.00 32.12 326 **ATOM** 1290 O SER 326 56.590 25.574 26.240 1.00 30.91 **ATOM** 1291 N THR 327 57.276 23.464 26.583 1.00 35.41 ATOM 1292 CA THR 327 56.420 23.278 27.747 1.00 39.61 **ATOM** 1293 CB THR 327 55.777 21.890 27.758 1.00 38.84 **ATOM** 1294 OG1 THR 327 56.784 20.890 27.538 1.00 42.53 **ATOM** 1295 CG2 THR 327 54.716 21.802 26.679 1.00 40.78 **ATOM** 1296 C THR 327 57.232 23.471 29.022 1.00 43.86 **ATOM** 1297 O THR 327 56.785 23.133 30.118 1.00 42.40 ATOM 1298 N **ASP** 328 58.417 24.054 28.869 1.00 47.35 1299 CA ASP **ATOM** 328 59.309 24.308 29.987 1.00 49.43 ATOM 1300 CB ASP 328 60.750 24.358 29.482 1.00 58.03 **ATOM** 1301 CG ASP 328 61.718 23.687 30.425 1.00 72.16 **ATOM** 1302 OD1 ASP 328 61.816 24.117 31.595 1.00 82.32 ATOM 1303 OD2 ASP 328 62.378 22.720 29.994 1.00 81.63 ATOM 1304 C **ASP** 328 58.951 25.625 30.676 1.00 47.99 **ATOM** 1305 O **ASP** 328 59.830 26.373 31.093 1.00 53.33 **ATOM** 1306 N **ARG** 329 57.657 25.910 30.780 1.00 48.33 ATOM 1307 CA ARG 329 57.177 27.135 31.413 1.00 47.67 **ATOM** 1308 CB ARG 329 56.562 28.091 30.379 1.00 47.64 **ATOM** 1309 CG ARG 329 57.550 28.802 29.450 1.00 47.87 **ATOM** 1310 CD ARG 329 57.893 27.968 28.226 1.00 44.00 **ATOM** 1311 NE ARG 329 58.759 28.682 27.288 1.00 41.17 **ATOM** 1312 CZ ARG 329 60.087 28.605 27.283 1.00 48.58 **ATOM** 329 1313 NH1 ARG 60.719 27.848 28.172 1.00 52.94 **ATOM** 1314 NH2 ARG 329 60.784 29.257 26.362 1.00 43.16 56.126 26.778 32.457 1.00 48.01 **ATOM** 1315 C ARG 329 ATOM 1316 O ARG 329 55.573 25.677 32.437 1.00 50.22 **ATOM** 1317 N SER 330 55.832 27.716 33.351 1.00 47.37 330 54.848 27.490 34.402 1.00 47.64 **ATOM** 1318 CA SER **ATOM** 1319 CB SER 330 55.376 28.021 35.736 1.00 46.62 **ATOM** 1320 C SER 330 53.506 28.139 34.074 1.00 46.40

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ATOM		53.460 29.252 33.548 1.00 48.49
ATOM	1322 N GLY 331	52.421 27.424 34.359 1.00 44.16
ATOM	1323 CA GLY 331	51.090 27.956 34.123 1.00 41.44
ATOM	1324 C GLY 331	50.424 27.660 32.790 1.00 42.83
ATOM		49.478 28.351 32.413 1.00 45.88
ATOM	1326 N- LEU 332	50.889 26.643 32.075 1.00 40.10
ATOM	1327 CA LEU 332	50.288 26.300 30.789 1.00 39.27
ATOM		51.301 25.596 29.885 1.00 37.42
ATOM	1329 CG LEU 332	52.436 26.426 29.291 1.00 35.35
ATOM	1330 CD1 LEU 332	53.374 25.505 28.530 1.00 31.61
ATOM	1331 CD2 LEU 332	51.875 27.511 28.376 1.00 31.82
ATOM	1332 C LEU 332	49.058 25.415 30.951 1.00 39.32
ATOM	1333 O LEU 332	49.060 24.467 31.738 1.00 42.74
ATOM	1334 N LEU 333	48.009 25.730 30.202 1.00 37.62
ATOM	1335 CA LEU 333	46.778 24.953 30.241 1.00 41.30
ATOM	1336 CB LEU 333	45.586 25.835 29.852 1.00 43.52
ATOM	1337 CG LEU 333	45.125 26.904 30.848 1.00 49.39
ATOM	1338 CD1 LEU 333	44.296 27.970 30.142 1.00 46.19
ATOM	1339 CD2 LEU 333	44.330 26.248 31.968 1.00 51.29
ATOM	1340 C LEU 333	46.859 23.762 29.285 1.00 41.39
ATOM	1341 O LEU 333	46.565 22.628 29.657 1.00 43.41
ATOM	1342 N CYA 334	47.317 24.024 28.067 1.00 42.18
ATOM	1343 CA CYA 334	47.409 23.003 27.029 1.00 39.56
ATOM	1344 CB CYA 334	47.004 23.616 25.691 1.00 45.48
ATOM '	1345 SG CYA 334	45.517 24.616 25.785 1.00 51.57
ATOM	1346 AS CYA 334	44.187 22.808 25.555 1.00 90.90
ATOM	1347 C CYA 334	48.776 22.347 26.891 1.00 38.28
ATOM	1348 O CYA 334	49.273 22.178 25.778 1.00 40.95
ATOM	1349 N VAL 335	49.345 21.913 28.009 1.00 36.05
ATOM	1350 CA VAL 335	50.661 21.278 28.006 1.00 35.78
ATOM	1351 CB VAL 335	50.996 20.679 29.399 1.00 35.53
ATOM	1352 CG1 VAL 335	52.413 20.123 29.407 1.00 32.76
ATOM	1353 CG2 VAL 335	50.822 21.729 30.490 1.00 28.87
ATOM	1354 C VAL 335	50.776 20.170 26.950 1.00 36.41
ATOM	1355 O VAL 335	51.756 20.104 26:202 1.00 34.26
ATOM	1356 N ASP 336	49.756 19.323 26.880 1.00 38.42
ATOM	1357 CA ASP 336	49.736 18.209 25.942 1.00 39.71
ATOM	1358 CB ASP 336	48.485 17.359 26.179 1.00 51.53
ATOM	1359 CG ASP 336	48.534 16.028 25.452 1.00 65.98
ATOM	1360 OD1 ASP 336	49.240 15.114 25.934 1.00 70.75
ATOM	1361 OD2 ASP 336	47.858 15.891 24.406 1.00 72.15
ATOM	1362 C ASP 336	49.794 18.668 24.486 1.00 37.72
ATOM	1363 O ASP 336	50.686 18.259 23.733 1.00 32.08
ATOM	1364 N LYS 337	48.858 19.532 24.100 1.00 33.78
ATOM	1365 CA LYS 337	48.797 20.040 22.731 1.00 28.00
ATOM	1366 CB LYS 337	47.626 21.022 22.574 1.00 22.46
ATOM	1367 C LYS 337	50.116 20.704 22.334 1.00 29.06

ATOM 1368 O LYS 337 50.607 20.512 21.220 1.00 28.41 **ATOM** 1369 N ILE 338 50.705 21.449 23.267 1.00 27.56 1370 CA ILE **ATOM** 338 51.964 22.138 23.022 1.00 25.03 ATOM 1371 CB ILE 338 52.274 23.149 24.144 1.00 19.49 1372 CG2 ILE ATOM 338 53.577 23.876 23.859 1.00 19.00 ATOM 1373 CG1 ILE 338 51.135 24.167 24.232 1.00 21.97 **ATOM** 1374 CD1 ILE 338 51.277 25.175 25.348 1.00 26.67 ATOM 1375 C ILE 338 53.119 21.153 22.826 1.00 29.97 ATOM 1376 O ILE 338 53.935 21.328 21.914 1.00 31.00 **ATOM** 1377 N GLU 339 53.165 20.100 23.642 1.00 33.52 ATOM 1378 CA GLU 339 54.213 19.080 23.516 1.00 35.34 1379 CB GLU 339 **ATOM** 54.136 18.062 24.659 1.00 39.97 1380 CG GLU 339 ATOM 54.653 18.585 25.986 1.00 53.23 **ATOM** 1381 CD GLU 339 54.549 17.579 27.126 1.00 61.16 **ATOM** 1382 OE1 GLU 339 53.602 16.759 27.131 1.00 64.30 1383 OE2 GLU 339 **ATOM** 55.412 17.622 28.031 1.00 57.76 ATOM 1384 C GLU 339 54.091 18.353 22.178 1.00 31.63 ATOM 1385 O GLU 339 55.086 18.123 21.491 1.00 28.96 **ATOM** 1386 N LYS 340 52.861 18.006 21.810 1.00 30.95 ATOM 1387 CA LYS 52.602 17.313 20.554 1.00 31.58 340 **ATOM** 1388 CB LYS 340 51.121 16.966 20.438 1.00 31.83 1389 C LYS 340 **ATOM** 53.057 18.159 19.358 1.00 29.84 **ATOM** 1390 O LYS 340 53.696 17.640 18.438 1.00 31.58 1391 N SER 341 ATOM 52.765 19.460 19.388 1.00 25.33 **ATOM** 1392 CA SER 341 53.165 20.351 18.297 1.00 23.92 **ATOM** 1393 CB SER 341 52.468 21.707 18.400 1.00 24.02 341 1394 OG SER ATOM 52.700 22.302 19.657 1.00 48.88 **ATOM** 1395 C SER 341 54.677 20.533 18.240 1.00 24.39 **ATOM** 1396 O SER 341 55.254 20.593 17.150 1.00 24.71 **ATOM** 1397 N GLN 342 55.324 20.606 19.405 1.00 25.45 **ATOM** 1398 CA GLN 342 56.777 20.751 19.437 1.00 26.66 **ATOM** 1399 CB GLN 342 57.311 20.975 20.853 1.00 22.77 **ATOM** 1400 CG GLN 342 58.805 21.307 20.840 1.00 25.76 1401 CD GLN ATOM 342 59.427 21.371 22.214 1.00 28.46 1402 OE1 GLN 342 ATOM 59.342 20.422 22.990 1.00 34.22 **ATOM** 1403 NE2 GLN 342 60.080 22.483 22.517 1.00 30.01 **ATOM** 1404 C GLN 342 57.425 19.504 18.843 1.00 23.37 **ATOM** 1405 O GLN 342 58.414 19.598 18.106 1.00 23.65 **ATOM** 1406 N GLU 343 56.864 18.340 19.162 1.00 21.48 1407 CA GLU 343 57.370 17.076 18.641 1.00 20.74 **ATOM ATOM** 1408 CB GLU 343 56.599 15.902 19.247 1.00 22.09 **ATOM** 1409 C GLU 343 57.225 17.094 17.119 1.00 19.18 58.156 16.743 16.393 1.00 21.11 1410 O GLU 343 ATOM 56.077 17.570 16.648 1.00 19.93 **ATOM** 1411 N ALA 344 ATOM 1412 CA ALA 344 55.803 17.662 15.217 1.00 20.20 54.411 18.216 14.989 1.00 16.46 1413 CB ALA 344 ATOM 1414 C ALA 344 56.850 18.539 14.528 1.00 20.75 **ATOM**

ATOM 1415 O ALA 344 57.432 18.140 13.514 1.00 25.13 ATOM 1416 N TYR 345 57.105 19.722 15.088 1.00 21.31 **ATOM** 1417 CA TYR 345 58.107 20.631 14.531 1.00 15.93 **ATOM** 1418 CB TYR 58.127 21.969 15.282 1.00 17.29 345 **ATOM** 1419 CG TYR 345 57.049 22.927 14.833 1.00 16.11 **ATOM** 1420 CD1 TYR 345 56.017 23.296 15.689 1.00 9.93 ATOM 1421 CE1 TYR 345 54.999 24.138 15.263 1.00 16.95 **ATOM** 1422 CD2 TYR 345 57.041 23.431 13.531 1.00 19.84 1423 CE2 TYR ATOM 345 56.026 24.276 13.094 1.00 17.13 ATOM 1424 CZ TYR 345 55.005 24.622 13.963 1.00 18.12 ATOM 1425 OH TYR 345 53.980 25.430 13.530 1.00 26.25 **ATOM** 1426 C TYR 345 59.493 20.008 14.554 1.00 20.65 60.240 20.129 13.583 1.00 20.75 ATOM 1427 O TYR 345 1428 N LEU **ATOM** 346 59.832 19.337 15.655 1.00 22.14 ATOM 1429 CA LEU 346 61.134 18.684 15.803 1.00 19.43 1430 CB LEU 61.267 18.041 17.186 1.00 19.92 ATOM 346 **ATOM** 1431 CG LEU 346 61.683 18.945 18.347 1.00 25.56 **ATOM** 1432 CD1 LEU 346 61.440 18.244 19.677 1.00 22.06 **ATOM** 1433 CD2 LEU 346 63.147 19.332 18.197 1.00 17.62 **ATOM** 1434 C LEU 346 61.359 17.635 14.723 1.00 19.30 **ATOM** 1435 O LEU 346 62.441 17.560 14.142 1.00 22.84 **ATOM** 1436 N LEU 347 60.337 16.826 14.456 1.00 25.17 **ATOM** 1437 CA LEU 347 60.423 15.790 13.427 1.00 24.55 ATOM 1438 CB LEU 347 59.187 14.892 13.453 1.00 25.47 **ATOM** 1439 CG LEU 347 59.256 13.654 14.345 1.00 30.65 ATOM 1440 CD1 LEU 347 57.941 12.890 14.258 1.00 34.28 **ATOM** 1441 CD2 LEU 347 60.416 12.765 13.908 1.00 28.26 **ATOM** 1442 C LEU 347 60.584 16.400 12.042 1.00 24.00 **ATOM** 1443 O LEU 347 61.399 15.932 11.245 1.00 29.74 1444 N ALA **ATOM** 348 59.809 17.443 11.761 1.00 22.72 1445 CA ALA 348 **ATOM** 59.875 18.125 10.475 1.00 19.19 1446 CB ALA 348 **ATOM** 58.789 19.188 10.388 1.00 22.73 **ATOM** 1447 C ALA 348 61.246 18.762 10.316 1.00 20.34 **ATOM** 1448 O ALA 348 61.881 18.633 9.274 1.00 23.94 **ATOM** 1449 N PHE 349 61.707 19.402 11.388 1.00 22.19 1450 CA PHE 349 **ATOM** 63.001 20.078 11.435 1.00 19.41 **ATOM** 1451 CB PHE 349 63.185 20.701 12.832 1.00 17.45 349 ATOM 1452 CG PHE 64.371 21.632 12.963 1.00 18.70 349 **ATOM** 1453 CD1 PHE 65.183 21.943 11.874 1.00 19.09 1454 CD2 PHE 349 ATOM 64.669 22.203 14.199 1.00 21.81 **ATOM** 1455 CE1 PHE 349 66.270 22.811 12.012 1.00 21.49 1456 CE2 PHE 349 65.753 23.072 14.351 1.00 18.58 **ATOM ATOM** 1457 CZ PHE 349 66.555 23.376 13.256 1.00 18.67 ATOM 1458 C PHE 349 64.110 19.071 11.136 1.00 20.96 **ATOM** 1459 O PHE 349 64.967 19.311 10.283 1.00 25.19 1460 N GLU 350 ATOM 64.076 17.935 11.824 1.00 23.96 **ATOM** 1461 CA GLU 350 65.077 16.888 11.642 1.00 27.98

ATOM	1 1462 CB GLU 350	64.794 15.721 12.591 1.00 28.90
ATOM	1 1463 CG GLU 350	65.738 14.542 12.413 1.00 39.36
ATOM	1464 CD GLU 350	65.603 13.497 13.505 1.00 41.62
ATOM	1465 OE1 GLU 350	64.475 13.260 13.988 1.00 43.67
ATOM	1466 OE2 GLU 350	66.636 12.908 13.876 1.00 49.64
ATOM	1467 C- GLU 350	65.100 16.385 10.203 1.00 27.12
ATOM	1468 O GLU 350	66.158 16.288 9.577 1.00 27.44
ATOM	1469 N HIS 351	63.918 16.088 9.678 1.00 27.36
ATOM	1470 CA HIS 351	63.787 15.591 8.318 1.00 23.97
ATOM	1471 CB HIS 351	62.366 15.087 8.090 1.00 22.89
ATOM	1472 CG HIS 351	61.991 13.945 8.986 1.00 24.58
ATOM	1473 CD2 HIS 351	62.736 13.209 9.846 1.00 25.83
ATOM	1474 ND1 HIS 351	60.709 13.448 9.073 1.00 26.50
ATOM	1475 CE1 HIS 351	60.677 12.460 9.948 1.00 24.81
ATOM	1476 NE2 HIS 351	61.896 12.295 10.431 1.00 28.42
ATOM	1477 C HIS 351	64.200 16.635 7.278 1.00 24.22
ATOM	1478 O HIS 351	64.757 16.287 6.236 1.00 25.79
ATOM	1479 N TYR 352	63.969 17.912 7.572 1.00 21.04
ATOM		64.363 18.974 6.654 1.00 18.98
ATOM	1481 CB TYR 352	63.770 20.321 7.067 1.00 17.08
ATOM	1482 CG TYR 352	64.127 21.413 6.090 1.00 21.83
ATOM	1483 CD1 TYR 352	63.537 21.467 4.828 1.00 20.07
ATOM	1484 CE1 TYR 352	63.941 22.411 3.883 1.00 23.51
ATOM	1485 CD2 TYR 352	65.121 22.339 6.388 1.00 19.94
ATOM	1486 CE2 TYR 352	65.531 23.284 5.452 1.00 20.85
ATOM	1487 CZ TYR 352	64.942 23.313 4.203 1.00 24.80
ATOM	1488 OH TYR 352	65.380 24.221 3.269 1.00 26.74
ATOM	1489 C TYR 352	65.889 19.055 6.624 1.00 20.58
ATOM	1490 O TYR 352	66.492 19.276 5.570 1.00 22.72
ATOM	1491 N VAL 353	66.508 18.877 7.789 1.00 28.34
ATOM ATOM	1492 CA VAL 353	67.967 18.892 7.904 1.00 22.38
ATOM	1493 CB VAL 353	68.419 18.755 9.389 1.00 26.46
ATOM	1494 CG1 VAL 353 1495 CG2 VAL 353	69.915 18.527 9.478 1.00 20.92
ATOM	1496 C VAL 353	68.053 20.009 10.165 1.00 22.46 68.518 17.725 7.078 1.00 23.51
ATOM	1497 O VAL 353	69.535 17.865 6.391 1.00 24.73
ATOM	1498 N ASN 354	67.850 16.575 7.158 1.00 20.93
ATOM	1499 CA ASN 354	68.252 15.392 6.397 1.00 27.25
ATOM	1500 CB ASN 354	67.320 14.210 6.680 1.00 28.43
ATOM	1501 CG ASN 354	67.521 13.607 8.058 1.00 28.43
ATOM	1502 OD1 ASN 354	68.565 13.787 8.692 1.00 37.79
ATOM	1503 ND2 ASN 354	66.521 12.867 8.524 1.00 26.44
ATOM	1504 C ASN 354	68.182 15.721 4.908 1.00 31.27
ATOM	1505 O ASN 354	69.066 15.347 4.134 1.00 34.22
ATOM		67.124 16.429 4.520 1.00 30.49
ATOM	1507 CA HIS 355	66.917 16.826 3.132 1.00 26.88
ATOM	1508 CB HIS 355	65.548 17.494 2.975 1.00 27.27
		2.575 1.00 27.27

1509 CG HIS 65.319 18.103 1.625 1.00 37.76 ATOM 355 ATOM 1510 CD2 HIS 355 65.439 19.382 1.196 1.00 35.28 ATOM 1511 ND1 HIS 355 64.913 17.369 0.532 1.00 34.93 **ATOM** 1512 CE1 HIS 355 64.789 18.169 -0.513 1.00 34.84 ATOM 1513 NE2 HIS 355 65.104 19.394 -0.135 1.00 33.13 **ATOM** 1514 C- HIS 355 68.016 17.748 2.610 1.00 24.66 ATOM 1515 O HIS 355 68.420 17.630 1.456 1.00 26.62 ATOM 1516 N ARG 356 68.487 18.670 3.448 1.00 25.86 1517 CA ARG 69.536 19.608 3.040 1.00 26.94 ATOM 356 ATOM 1518 CB ARG 356 69.620 20.791 3.996 1.00 20.57 **ATOM** 1519 CG ARG 356 68.453 21.727 3.899 1.00 19.69 **ATOM** 1520 CD ARG 356 68.866 23.110 4.340 1.00 23.81 **ATOM** 1521 NE ARG 356 69.768 23.746 3.388 1.00 23.14 ATOM 1522 CZ ARG 356 70.641 24.697 3.702 1.00 24.11 **ATOM** 1523 NH1 ARG 356 70.755 25.129 4.949 1.00 26.29 **ATOM** 1524 NH2 ARG 356 71.384 25.242 2.754 1.00 32.79 **ATOM** 1525 C ARG 356 70.921 19.002 2.875 1.00 29.38 ATOM 1526 O ARG 356 71.795 19.607 2.257 1.00 32.91 **ATOM** 1527 N LYS 357 71.133 17.848 3.498 1.00 33.39 **ATOM** 1528 CA LYS 357 72.401 17.128 3.417 1.00 35.97 1529 CB LYS 357 ATOM 72.479 16.363 2.089 1.00 40.55 ATOM 1530 CG LYS 357 71.327 15.381 1.891 1.00 44.03 1531 CD LYS 357 ATOM 0.523 1.00 52.31 71.360 14.722 ATOM 1532 CE LYS 357 70.171 13.787 0.343 1.00 56.99 ATOM 1533 NZ LYS 357 70.208 13.085 -0.970 1.00 64.78 **ATOM** 1534 C LYS 357 73.657 17.981 3.629 1.00 38.55 1535 O LYS **ATOM** 357 74.518 18.079 2.748 1.00 42.50 **ATOM** 1536 N HIS 358 73.751 18.601 4.802 1.00 35.00 1537 CA HIS 358 **ATOM** 74.906 19.418 5.155 1.00 32.94 1538 CB HIS 358 ATOM 74.732 20.018 6.552 1.00 27.62 **ATOM** 1539 CG HIS 358 73.669 21.067 6.643 1.00 26.64 72.330 20.968 **ATOM** 1540 CD2 HIS 358 6.819 1.00 20.85 73.950 22.416 6.587 1.00 24.71 **ATOM** 1541 ND1 HIS 358 1542 CE1 HIS ATOM 358 72.831 23.103 6.724 1.00 21.02 **ATOM** 1543 NE2 HIS 358 71.834 22.248 6.865 1.00 21.42 **ATOM** 1544 C HIS 358 76.140 18.520 5.176 1.00 36.60 **ATOM** 1545 O HIS 358 76.072 17.379 5.635 1.00 38.73 1546 N ASN 359 **ATOM** 77.267 19.037 4.702 1.00 41.40 1547 CA ASN **ATOM** 359 78.515 18.277 4.689 1.00 45.02 **ATOM** 1548 CB ASN 359 79.441 18.799 3.587 1.00 42.57 1549 C ASN 359 **ATOM** 79.193 18.386 6.058 1.00 46.59 ASN **ATOM** 1550 O 359 80.405 18.588 6.150 1.00 52.31 **ATOM** 1551 N ILE 360 78.400 18.254 7.117 1.00 45.14 **ATOM** 1552 CA ILE 360 78.896 18.348 8.487 1.00 43.69 **ATOM** 1553 CB ILE 360 78.330 19.597 9.207 1.00 40.08 1554 CG2 ILE **ATOM** 360 78.824 19.657 10.645 1.00 32.11 **ATOM** 1555 CG1 ILE 360 78.733 20.864 8.452 1.00 41.47

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ATOM	1556 CD1 ILE 360	78.057 22.115 8.954 1.00 44.93
ATOM	1557 C ILE 360	78.452 17.101 9.242 1.00 43.63
ATOM	1558 O ILE 360	77.257 16.797 9.313 1.00 45.20
ATOM	1559 N PRO 361	79.413 16.337 9.780 1.00 43.91
ATOM	1560 CD PRO 361	80.871 16.540 9.699 1.00 47.07
ATOM	1561 CA PRO 361	79.087 15.118 10.526 1.00 41.66
ATOM	1562 CB PRO 361	80.462 14.495 10.782 1.00 43.73
ATOM	1563 CG PRO 361	81.383 15.679 10.830 1.00 45.45
ATOM	1564 C PRO 361	78.332 15.403 11.832 1.00 36.42
ATOM	1565 O PRO 361	78.679 16.325 12.572 1.00 35.74
ATOM	1566 N HIS 362	77.291 14.610 12.088 1.00 33.14
ATOM	1567 CA HIS 362	76.462 14.726 13.292 1.00 34.09
ATOM	1568 CB HIS 362	77.288 14.413 14.547 1.00 33.82
ATOM	1569 CG HIS 362	78.132 13.181 14.424 1.00 36.04
ATOM	1570 CD2 HIS 362	77.793 11.885 14.224 1.00 34.77
ATOM	1571 ND1 HIS 362	79.509 13.212 14.482 1.00 37.16
ATOM	1572 CE1 HIS 362	79.983 11.990 14.325 1.00 37.16
ATOM	1573 NE2 HIS 362	78.962 11.165 14.167 1.00 40.13
ATOM	1574 C HIS 362	75.829 16.110 13.417 1.00 31.00
ATOM	1575 O HIS 362	75.617 16.608 14.525 1.00 30.22
ATOM	1576 N PHE 363	75.478 16.690 12.272 1.00 33.06
ATOM	1577 CA PHE 363	74.878 18.021 12.200 1.00 28.08
ATOM	1578 CB PHE 363	74.503 18.355 10.747 1.00 25.26
ATOM	1579 CG PHE 363	73.923 19.733 10.567 1.00 24.91
ATOM	1580 CD1 PHE 363	74.750 20.817 10.320 1.00 27.60
ATOM ATOM	1581 CD2 PHE 363 1582 CE1 PHE 363	72.552 19.948 10.664 1.00 25.52
ATOM	1582 CE1 PHE 363 1583 CE2 PHE 363	74.221 22.100 10.175 1.00 29.70 72.014 21.227 10.522 1.00 25.88
ATOM	1584 CZ PHE 363	72.850 22.304 10.278 1.00 21.49
ATOM	1585 C PHE 363	73.659 18.201 13.099 1.00 23.79
ATOM	1586 O PHE 363	73.587 19.164 13.863 1.00 24.48
ATOM	1587 N TRP 364	72.707 17.277 13.012 1.00 23.13
ATOM	1588 CA TRP 364	71.484 17.369 13.805 1.00 25.06
ATOM	1589 CB TRP 364	70.536 16.201 13.494 1.00 21.17
ATOM	1590 CG TRP 364	69.247 16.220 14.271 1.00 23.14
ATOM	1591 CD2 TRP 364	68.261 17.266 14.296 1.00 27.68
ATOM	1592 CE2 TRP 364	67.229 16.845 15.165 1.00 28.31
ATOM	1593 CE3 TRP 364	68.149 18.517 13.671 1.00 26.46
ATOM	1594 CD1 TRP 364	68.784 15.241 15.096 1.00 23.76
ATOM	1595 NE1 TRP 364	67.576 15.607 15.637 1.00 32.12
ATOM	1596 CZ2 TRP 364	66.100 17.628 15.427 1.00 25.63
ATOM	1597 CZ3 TRP 364	67.028 19.294 13.931 1.00 25.55
ATOM	1598 CH2 TRP 364	66.017 18.845 14.803 1.00 29.79
ATOM	1599 C TRP 364	71.715 17.531 15.312 1.00 27.80
ATOM	1600 O TRP 364	71.212 18.486 15.904 1.00 26.96
ATOM	1601 N PRO 365	72.458 16.605 15.955 1.00 30.69
ATOM	1602 CD PRO 365	72.974 15.308 15.481 1.00 31.45

ATOM 1603 CA PRO 365 72.687 16.757 17.397 1.00 27.97 **ATOM** 1604 CB PRO 365 73.506 15.512 17.752 1.00 26.50 **ATOM** 1605 CG PRO 365 73.057 14.509 16.757 1.00 33.47 **ATOM** 1606 C PRO 365 73.457 18.043 17.709 1.00 27.10 **ATOM** 1607 O PRO 365 73.154 18.736 18.681 1.00 26.88 **ATOM** 1608 N- LYS 366 74.440 18.365 16.873 1.00 26.99 1609 CA LYS **ATOM** 366 75.230 19.577 17.061 1.00 30.69 ATOM 1610 CB LYS 76.275 19.708 15.957 1.00 28.53 366 ATOM 1611 CG LYS 366 77.481 18.804 16.106 1.00 28.89 **ATOM** 1612 CD LYS 366 78.430 19.027 14.939 1.00 32.51 **ATOM** 1613 CE LYS 366 79.743 18.294 15.116 1.00 38.52 **ATOM** 1614 NZ LYS 366 80.632 18.506 13.939 1.00 45.28 ATOM 1615 C LYS 74.349 20.831 17.079 1.00 36.18 366 **ATOM** 1616 O LYS 366 74.472 21.672 17.972 1.00 39.82 **ATOM** 1617 N LEU 367 73.464 20.950 16.091 1.00 37.54 **ATOM** 1618 CA LEU 367 72.557 22.092 15.994 1.00 36.14 **ATOM** 1619 CB LEU 367 71.803 22.070 14.659 1.00 32.20 **ATOM** 1620 CG LEU 367 70.764 23.179 14.447 1.00 36.16 **ATOM** 1621 CD1 LEU 367 71.402 24.567 14.618 1.00 20.60 **ATOM** 1622 CD2 LEU 367 70.139 23.030 13.065 1.00 34.30 **ATOM** 1623 C LEU 367 71.561 22.060 17.143 1.00 36.84 **ATOM** 1624 O LEU 367 71.231 23.091 17.729 1.00 36.94 **ATOM** 1625 N LEU 368 71.083 20.866 17.459 1.00 37.81 ATOM 1626 CA LEU 368 70.130 20.683 18.536 1.00 34.83 **ATOM** 1627 CB LEU 368 69.763 19.205 18.622 1.00 36.98 **ATOM** 1628 CG LEU 368 68.421 18.777 19.205 1.00 40.34 **ATOM** 1629 CD1 LEU 368 67.276 19.595 18.619 1.00 36.28 **ATOM** 1630 CD2 LEU 368 68.241 17.299 18.908 1.00 39.39 **ATOM** 1631 C LEU 368 70.755 21.182 19.843 1.00 38.32 **ATOM** 1632 O LEU 368 70.059 21.711 20.707 1.00 41.87 **ATOM** 1633 N MET 369 72.075 21.057 19.962 1.00 39.46 **ATOM** 1634 CA MET 369 72.790 21.515 21.154 1.00 40.12 **ATOM** 1635 CB MET 369 74.219 20.971 21.168 1.00 41.26 **ATOM** 1636 CG MET 369 74.307 19.493 21.521 1.00 47.83 **ATOM** 1637 SD MET 369 75.961 18.810 21.289 1.00 55.72 **ATOM** 1638 CE MET 369 76.809 19.474 22.727 1.00 54.37 **ATOM** 1639 C MET 369 72.805 23.039 21.251 1.00 42.81 369 **ATOM** 1640 O MET 72.990 23.601 22.335 1.00 47.81 1641 N LYS 370 **ATOM** 72.622 23.708 20.115 1.00 40.09 1642 CA LYS 370 72.588 25.165 20.080 1.00 33.65 **ATOM** 1643 CB LYS 370 **ATOM** 72.751 25.677 18.650 1.00 30.83 1644 CG LYS 370 **ATOM** 74.138 25.435 18.078 1.00 30.98 75.188 26.198 18.867 1.00 37.82 **ATOM** 1645 CD LYS 370 ATOM 1646 CE LYS 370 76.591 25.938 18.351 1.00 36.05 **ATOM** 1647 NZ LYS 370 77.034 24.562 18.667 1.00 48.68 **ATOM** 1648 C LYS 370 71.293 25.684 20.702 1.00 33.32 ATOM 1649 O LYS 370 71.218 26.842 21.112 1.00 34.75

ATOM 1650 N VAL 70.277 24.826 20.779 1.00 31.90 371 ATOM 1651 CA VAL 371 69.006 25.197 21.395 1.00 31.77 **ATOM** 1652 CB VAL 371 67.933 24.092 21.214 1.00 30.28 ATOM 1653 CG1 VAL 371 66.673 24.429 21.995 1.00 30.02 **ATOM** 1654 CG2 VAL 67.596 23.933 19.746 1.00 32.23 371 **ATOM** 1655 C- VAL 371 69.277 25.417 22.885 1.00 34.44 **ATOM** 1656 O VAL 371 68.722 26.331 23.499 1.00 33.35 372 ATOM 1657 N THR 70.161 24.590 23.443 1.00 33.15 1658 CA THR 372 ATOM 70.551 24.675 24.847 1.00 32.47 ATOM 1659 CB THR 372 71.541 23.556 25.207 1.00 32.11 **ATOM** 1660 OG1 THR 372 70.955 22.288 24.891 1.00 35.33 ATOM 1661 CG2 THR 372 71.894 23.603 26.688 1.00 32.54 **ATOM** THR 1662 C 372 71.226 26.020 25.108 1.00 34.49 1663 O ATOM THR 372 70.936 26.696 26.099 1.00 34.07 1664 N ASP 72.120 26.405 24.202 1.00 32.77 ATOM 373 **ATOM** 1665 CA ASP 373 72.830 27.671 24.315 1.00 28.08 **ATOM** 1666 CB ASP 373 73.803 27.841 23.147 1.00 31.59 **ATOM** 1667 CG ASP 373 74.910 26.789 23.142 1.00 37.29 ATOM 1668 OD1 ASP 373 75.170 26.169 24.196 1.00 40.82 **ATOM** 1669 OD2 ASP 373 75.531 26.586 22.079 1.00 40.81 **ATOM** 1670 C ASP 373 71.830 28.821 24.353 1.00 29.21 1671 O **ATOM** ASP 373 71.931 29.709 25.200 1.00 31.85 70.843 28.775 23.463 1.00 24.71 **ATOM** 1672 N LEU 374 **ATOM** 1673 CA LEU 374 69.813 29.802 23.403 1.00 25.25 **ATOM** 1674 CB LEU 374 68.906 29.587 22.188 1.00 25.61 ATOM 1675 CG LEU 374 69.480 30.084 20.858 1.00 25.51 ATOM 1676 CD1 LEU 374 68.741 29.469 19.677 1.00 23.53 ATOM 1677 CD2 LEU 374 69.405 31.596 20.820 1.00 21.92 68.994 29.827 24.686 1.00 26.84 ATOM 1678 C LEU 374 ATOM 1679 O LEU 374 68.591 30.895 25.151 1.00 28.96 **ATOM** 1680 N ARG 375 68.746 28.651 25.254 1.00 31.00 **ATOM** 1681 CA ARG 375 67.996 28.554 26.502 1.00 32.86 **ATOM** 1682 CB ARG 375 67.831 27.090 26.924 1.00 36.80 ATOM 1683 CG ARG 375 66.861 26.297 26.071 1.00 44.91 **ATOM** 1684 CD ARG 375 65.433 26.731 26.338 1.00 58.99 **ATOM** 1685 NE ARG 375 64.501 26.210 25.342 1.00 72.26 1686 CZ ARG 375 **ATOM** 63.909 25.020 25.404 1.00 77.46 **ATOM** 1687 NH1 ARG 375 64.147 24.201 26.422 1.00 80.94 1688 NH2 ARG **ATOM** 375 63.062 24.657 24.447 1.00 75.58 **ATOM** 1689 C ARG 375 68.771 29.317 27.570 1.00 32.27 **ATOM** 1690 O **ARG** 375 68.199 30.125 28.304 1.00 33.75 **ATOM** 1691 N MET 376 70.084 29.098 27.602 1.00 32.65 1692 CA MET 376 **ATOM** 70.967 29.753 28.560 1.00 35.83 **ATOM** 376 1693 CB MET 72.392 29.210 28.434 1.00 39.25 1694 CG MET ATOM 376 72.526 27.751 28.839 1.00 54.45 ATOM 1695 SD MET 376 74.245 27.212 28.944 1.00 73.93 **ATOM** 1696 CE MET 376 74.421 26.270 27.434 1.00 67.01

ATOM 1697 C **MET** 70.960 31.267 28.378 1.00 35.38 376 **ATOM** 1698 O **MET** 376 70.882 32.015 29.353 1.00 34.73 **ATOM** 1699 N ILE 377 71.038 31.716 27.129 1.00 32.51 **ATOM** 1700 CA ILE 377 71.016 33.142 26.816 1.00 26.55 **ATOM** 1701 CB ILE 377 71.182 33.370 25.299 1.00 24.84 **ATOM** 1702 CG2 ILE 377 70.817 34.797 24.923 1.00 26.63 **ATOM** 1703 CG1 ILE 377 72.616 33.038 24.890 1.00 20.66 ATOM 1704 CD1 ILE 377 72.872 33.104 23.409 1.00 20.74 ATOM 1705 C ILE 377 69.706 33.755 27.313 1.00 25.47 ATOM 1706 O ILE 377 69.696 34.848 27.881 1.00 29.99 ATOM 1707 N GLY 378 68.608 33.033 27.127 1.00 25.11 **ATOM** 1708 CA GLY 378 67.321 33.522 27.580 1.00 27.82 ATOM 1709 C GLY 378 67.279 33.613 29.095 1.00 30.90 66.749 34.579 29.651 1.00 31.19 **ATOM** 1710 O GLY 378 **ATOM** 1711 N ALA 379 67.851 32.611 29.761 1.00 31.62 **ATOM** 1712 CA ALA 379 67.896 32.547 31.223 1.00 30.74 ATOM 1713 CB ALA 379 68.433 31.198 31.671 1.00 30.82 **ATOM** 1714 C ALA 379 68.756 33.668 31.801 1.00 30.07 **ATOM** ALA 68.327 34.384 32.708 1.00 31.05 1715 O 379 **ATOM** 1716 N CYA 380 69.966 33.817 31.273 1.00 29.72 1717 CA CYA 380 ATOM 70.873 34.866 31.723 1.00 33.36 1718 CB CYA ATOM 380 72.201 34.809 30.963 1.00 38.31 73.249 33.407 31.386 1.00 50.99 **ATOM** 1719 SG CYA 380 **ATOM** 1720 AS CYA 380 74.982 33.655 29.929 1.00 70.37 **ATOM** 1721 C CYA 380 70.226 36.232 31.535 1.00 33.40 ATOM 1722 O 380 CYA 70.246 37.062 32.442 1.00 36.41 **ATOM** 1723 N HIS 381 69.615 36.456 30.374 1.00 32.55 **ATOM** 1724 CA HIS 381 68.965 37.734 30.114 1.00 26.41 **ATOM** 1725 CB HIS 381 68.434 37.811 28.681 1.00 20.89 **ATOM** 1726 CG HIS 381 67.593 39.023 28.423 1.00 15.78 **ATOM** 1727 CD2 HIS 381 67.928 40.277 28.041 1.00 12.67 **ATOM** 1728 ND1 HIS 381 66.226 39.031 28.605 1.00 17.88 **ATOM** 1729 CE1 HIS 381 65.756 40.239 28.353 1.00 16.27 **ATOM** 1730 NE2 HIS 381 66.768 41.013 28.008 1.00 17.18 **ATOM** 1731 C HIS 381 67.839 38.023 31.102 1.00 26.73 1732 O HIS 381 **ATOM** 67.621 39.176 31.464 1.00 30.46 ATOM 1733 N ALA 382 67.111 36.991 31.521 1.00 26.68 1734 CA ALA 382 **ATOM** 66.010 37.176 32.464 1.00 27.90 **ATOM** 1735 CB ALA 382 65.237 35.878 32.642 1.00 25.29 **ATOM** 1736 C ALA 382 66.511 37.697 33.810 1.00 31.23 1737 O ALA 382 **ATOM** 65.927 38.617 34.378 1.00 37.67 **ATOM** 1738 N SER 383 67.596 37.114 34.316 1.00 34.15 383 68.174 37.550 35.588 1.00 37.23 **ATOM** 1739 CA SER **ATOM** 1740 CB SER 383 69.294 36.605 36.027 1.00 40.21 68.785 35.324 36.361 1.00 53.99 ATOM 1741 OG SER 383 **ATOM** 1742 C SER 383 68.727 38.958 35.417 1.00 33.67 68.532 39.827 36.268 1.00 40.73 **ATOM** 1743 O SER 383

	ATOM	1744 N ARG	384 69.41	11 39.171 34.298 1.00 29.95
	ATOM	1745 CA ARG	384 70.0	
	ATOM	1746 CB ARG	384 70.6	
	ATOM	1747 CG ARG	384 71.4	
	ATOM	1748 CD ARG	384 72.7	02.207
	ATOM	1749 NE ARG	384 73.6	57 42.660 32.358 1.00 41.68
٠	ATOM	1750 CZ ARG	384 74.58	
	ATOM	1751 NH1 ARG	384 74.7	
	ATOM	1752 NH2 ARG	384 75.3	49 44.213 32.455 1.00 37.27
	ATOM	1753 C ARG 3	384 68.91°	0 41.536 33.911 1.00 35.72
	ATOM	1754 O ARG 3	384 69.09	0 42.635 34.439 1.00 41.66
	ATOM	1755 N PHE 3	85 67.768	8 41.196 33.318 1.00 34.30
	ATOM	1756 CA PHE	385 66.64	6 42.119 33.199 1.00 32.40
	ATOM		385 65.52	7 41.502 32.356 1.00 29.02
	ATOM			4 42.407 32.163 1.00 26.56
	ATOM			17 43.320 31.119 1.00 26.59
	ATOM			63 42.355 33.037 1.00 24.69
	ATOM			1 44.173 30.947 1.00 31.70
	ATOM		385 62.17	
	ATOM			8 44.115 31.827 1.00 31.59
	ATOM		85 66.121	
	ATOM		85 65.822	
	ATOM			41.499 35.456 1.00 33.91
	ATOM ATOM		386 65.53°	
	ATOM		86 65.54° 886 64.32°	
	ATOM			
	ATOM			2 38.147 38.099 1.00 51.12 5 40.148 38.246 1.00 49.17
	ATOM			42.761 37.475 1.00 38.95
	ATOM		36 65.979	
	ATOM	1774 N HIS 38		42.613 37.248 1.00 33.62
	ATOM	1775 CA HIS 38		43.531 37.808 1.00 39.73
4	ATOM			42.980 37.639 1.00 40.71
	ATOM			41.749 38.449 1.00 52.03
4	ATOM	1778 CD2 HIS 38		40.967 39.181 1.00 53.85
4	ATOM	1779 ND1 HIS 38		41.189 38.566 1.00 54.79
4	ATOM	1780 CE1 HIS 38		40.114 39.334 1.00 56.55
4	ATOM	1781 NE2 HIS 38	70.336	39.958 39.720 1.00 57.48
1	ATOM	1782 C HIS 387	68.594	44.913 37.175 1.00 42.08
	ATOM	1783 O HIS 387	68.712	45.926 37.865 1.00 44.12
	MOTA			44.957 35.874 1.00 42.38
	ATOM	1785 CA MET 3	88 68.154	46.229 35.175 1.00 38.00
	ATOM			46.006 33.692 1.00 40.21
		1787 CG MET 3		45.555 32.829 1.00 41.26
				45.427 31.089 1.00 45.51
	ATOM			43.802 30.645 1.00 42.40
P	MOTA	1790 C MET 38	8 67.025	47.044 35.810 1.00 38.11

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ATOM	1791	O MET	388	67.155 48.255 35.997 1.00 38.41
ATOM	1792	N LYS	389	65.926 46.374 36.144 1.00 39.67
ATOM		CA LYS	389	64.773 47.036 36.750 1.00 44.96
ATOM		CB LYS	389	63.570 46.087 36.818 1.00 49.52
ATOM		CG LYS	389	62.674 46.102 35.588 1.00 56.74
ATOM		CD LYS	389	62.145 47.509 35.278 1.00 68.05
ATOM		CE LYS	389	61.287 48.100 36.403 1.00 71.47
ATOM		NZ LYS	389	60.038 47.330 36.661 1.00 71.98
ATOM		C LYS	389	65.041 47.604 38.141 1.00 46.60
ATOM		O LYS	389	64.516 48.661 38.499 1.00 47.25
ATOM		N VAL	390	65.832 46.893 38.935 1.00 47.15
ATOM		CA VAL	390	66.129 47.353 40.284 1.00 50.75
ATOM		CB VAL	390	66.686 46.202 41.182 1.00 50.42
ATOM		CG1 VAL	390	68.095 45.802 40.770 1.00 47.93
ATOM		CG2 VAL	390	66.650 46.612 42.640 1.00 56.67
ATOM ATOM	. •		390 390	67.072 48.558 40.286 1.00 49.82 66.971 49.426 41.152 1.00 52.44
ATOM		N GLU	391	66.971 49.426 41.152 1.00 52.44 67.926 48.651 39.272 1.00 46.14
ATOM		CA GLU	391	68.888 49.741 39.173 1.00 43.84
ATOM		CB GLU	391	70.150 49.268 38.449 1.00 41.44
ATOM		CG GLU	391	70.837 48.074 39.095 1.00 51.12
ATOM		CD GLU	391	71.218 48.325 40.540 1.00 57.29
ATOM		DE1 GLU	391	71.970 49.287 40.802 1.00 58.15
ATOM		E2 GLU	391	70.764 47.559 41.416 1.00 62.51
ATOM	1815 C	GLU	391	68.386 51.015 38.501 1.00 45.94
ATOM	1816 C) GLU	391	68.567 52.114 39.033 1.00 51.14
ATOM	1817 N	I CYA	392	67.727 50.872 37.354 1.00 45.84
ATOM	1818 C	CA CYA	392	67.255 52.029 36.598 1.00 41.60
ATOM		B CYA	392	67.681 51.889 35.140 1.00 42.06
ATOM		G CYA	392	69.452 52.008 34.968 1.00 44.47
ATOM		S CYA	392	69.867 50.812 33.150 1.00 54.22
ATOM	1822 C		392	65.779 52.395 36.683 1.00 42.27
ATOM	1823 C		392	64.937 51.564 37.029 1.00 43.91
ATOM	1824 N		393	65.451 53.674 36.414 1.00 42.79
ATOM	1825 C		393	66.384 54.774 36.106 1.00 38.59
ATOM ATOM			393 393	64.067 54.159 36.459 1.00 44.20 64.218 55.667 36.238 1.00 39.88
ATOM			393	64.218 55.667 36.238 1.00 39.88 65.487 55.789 35.459 1.00 35.88
ATOM	1829 C		393 193	63.178 53.513 35.398 1.00 45.29
ATOM	1830 O		393	63.600 53.308 34.257 1.00 43.97
ATOM	1831 N		394	61.935 53.238 35.782 1.00 48.20
ATOM			394	60.959 52.607 34.901 1.00 53.71
ATOM			394	59.605 52.429 35.629 1.00 59.59
ATOM			394	58.690 51.717 34.787 1.00 66.50
ATOM			394	59.013 53.787 36.004 1.00 61.00
ATOM	1836 C		94	60.752 53.358 33.581 1.00 51.35
	1837 O		94	60.419 52.751 32.563 1.00 54.39
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ATOM 1838 N GLU 395 61.008 54.664 33.595 1.00 47.65 **ATOM** 1839 CA GLU 395 60.845 55.509 32.414 1.00 44.43 **ATOM** 1840 CB GLU 395 60.988 56.978 32.804 1.00 43.85 **ATOM** 1841 C GLU 395 61.788 55.175 31.250 1.00 42.93 **ATOM** 1842 O GLU 395 61.589 55.649 30.129 1.00 41.39 **ATOM** 1843 N. LEU 396 62.818 54.375 31.517 1.00 39.38 **ATOM** 1844 CA LEU 396 63.782 53.989 30.486 1.00 35.70 ATOM 1845 CB LEU 396 65.185 53.867 31.090 1.00 34.96 1846 CG LEU **ATOM** 396 65.854 55.141 31.609 1.00 36.47 **ATOM** 1847 CD1 LEU 396 67.234 54.807 32.150 1.00 34.21 **ATOM** 1848 CD2 LEU 396 65.959 56.164 30.491 1.00 32.74 **ATOM** 1849 C LEU 396 63.407 52.671 29.803 1.00 34.60 **ATOM** LEU 1850 O 396 64.086 52.223 28.873 1.00 30.36 **ATOM** 1851 N PHE 397 62.325 52.059 30.269 1.00 33.02 **ATOM** 1852 CA PHE 397 61.868 50.792 29.725 1.00 33.39 ATOM 1853 CB PHE 397 61.615 49.782 30.852 1.00 34.30 ATOM 1854 CG PHE 397 62.834 49.439 31.665 1.00 32.62 **ATOM** 1855 CD1 PHE 397 63.296 50.301 32.654 1.00 32.35 ATOM 1856 CD2 PHE 397 63.504 48.241 31.461 1.00 31.28 **ATOM** 1857 CE1 PHE 397 64.407 49.976 33.426 1.00 27.01 **ATOM** 1858 CE2 PHE 397 64.616 47.905 32.229 1.00 33.34 **ATOM** 1859 CZ PHE 397 65.067 48.775 33.213 1.00 31.29 **ATOM** 1860 C PHE 397 60.580 50.961 28.934 1.00 33.17 **ATOM** 1861 O PHE 397 59.540 51.318 29.498 1.00 31.99 **ATOM** 1862 N PRO 398 60.636 50.752 27.606 1.00 32.45 **ATOM** 1863 CD PRO 398 61.821 50.493 26.768 1.00 28.15 **ATOM** 1864 CA PRO 398 59.429 50.885 26.786 1.00 30.02 ATOM 1865 CB PRO 398 59.921 50.483 25.394 1.00 28.15 **ATOM** 1866 CG PRO 398 61.352 50.923 25.397 1.00 24.89 **ATOM** 1867 C PRO 398 58.384 49.900 27.326 1.00 28.39 **ATOM** 1868 O PRO 398 58.735 48.810 27.789 1.00 28.00 **ATOM** 1869 N PRO 399 57.092 50.262 27.267 1.00 32.45 **ATOM** 1870 CD PRO 399 56.577 51.511 26.672 1.00 34.93 **ATOM** 1871 CA PRO 399 55.989 49.421 27.753 1.00 32.54 399 **ATOM** 1872 CB PRO 54.755 50.122 27.188 1.00 34.47 399 **ATOM** 1873 CG PRO 55.159 51.564 27.196 1.00 31.37 399 **ATOM** 1874 C PRO 56.044 47.946 27.338 1.00 32.18 **ATOM** 1875 O PRO 399 55.950 47.054 28.188 1.00 32.58 **ATOM** 1876 N LEU 400 56.195 47.689 26.041 1.00 30.15 **ATOM** 1877 CA LEU 400 56.259 46.314 25.541 1.00 32.32 **ATOM** 1878 CB LEU 400 56.211 46.297 24.011 1.00 28.67 **ATOM** 1879 CG LEU 400 56.028 44.927 23.351 1.00 28.77 1880 CD1 LEU 400 54.802 44.234 23.919 1.00 22.73 **ATOM** 1881 CD2 LEU **ATOM** 400 55.897 45.096 21.846 1.00 27.89 **ATOM** 1882 C LEU 400 57.496 45.561 26.051 1.00 32.27 **ATOM** 1883 O LEU 400 57.437 44.358 26.307 1.00 32.87 ATOM 1884 N PHE 401 58.602 46.279 26.215 1.00 32.27

ATOM 1885 CA PHE 401 59.847 45.695 26.710 1.00 32.39 **ATOM** 1886 CB PHE 401 60.946 46.769 26.711 1.00 31.38 **ATOM** 1887 CG PHE 401 62.290 46.286 27.194 1.00 35.12 **ATOM** 1888 CD1 PHE 401 62.835 45.089 26.729 1.00 34.68 **ATOM** 1889 CD2 PHE 401 63.030 47.051 28.097 1.00 34.57 **ATOM** 1890 CE1 PHE 401 64.100 44.662 27.155 1.00 30.27 **ATOM** 1891 CE2 PHE 401 64.291 46.635 28.526 1.00 33.57 1892 CZ PHE **ATOM** 64.828 45.438 28.054 1.00 35.74 401 ATOM 1893 C PHE 401 59.599 45.169 28.129 1.00 32.21 **ATOM** 1894 O PHE 401 60.002 44.056 28.478 1.00 33.36 **ATOM** 1895 N LEU 402 58.902 45.967 28.929 1.00 31.85 ATOM 1896 CA LEU 402 58.582 45.602 30.302 1.00 35.06 **ATOM** 1897 CB LEU 402 57.948 46.789 31.029 1.00 34.76 **ATOM** 1898 CG LEU 402 58.878 47.852 31.591 1.00 33.48 ATOM 1899 CD1 LEU 402 58.060 49.010 32.152 1.00 32.58 **ATOM** 1900 CD2 LEU 402 59.753 47.217 32.662 1.00 26.27 ATOM 1901 C LEU 402 57.626 44.426 30.393 1.00 36.80 **ATOM** 1902 O LEU 402 57.793 43.545 31.239 1.00 35.43 1903 N GLU ATOM 56.600 44.443 29.547 1.00 38.50 403 **ATOM** 1904 CA GLU 403 55.581 43.401 29.540 1.00 40.24 **ATOM** 1905 CB GLU 403 54.435 43.792 28.605 1.00 44.03 **ATOM** 1906 CG GLU 403 53.239 42.850 28.666 1.00 55.53 ATOM 1907 CD GLU 403 52.180 43.159 27.618 1.00 66.67 ATOM 1908 OE1 GLU 403 52.151 44.299 27.095 1.00 70.81 ATOM 1909 OE2 GLU 403 51.370 42.255 27.315 1.00 73.80 **ATOM** 56.096 42.018 29.162 1.00 38.00 1910 C GLU 403 **ATOM** 1911 O GLU 403 55.745 41.029 29.805 1.00 38.78 **ATOM** 1912 N VAL 404 56.934 41.955 28.132 1.00 37.39 **ATOM** 1913 CA VAL 404 57.475 40.686 27.652 1.00 37.05 1914 CB VAL 404 ATOM 58.180 40.855 26.286 1.00 35.57 **ATOM** 1915 CG1 VAL 404 58.677 39.513 25.776 1.00 36.85 1916 CG2 VAL **ATOM** 404 57.222 41.451 25.287 1.00 42.03 **ATOM** 1917 C VAL 404 58.438 40.000 28.609 1.00 38.69 **ATOM** 1918 O VAL 404 58.436 38.774 28.727 1.00 40.71 **ATOM** 1919 N PHE 405 59.267 40.785 29.286 1.00 39.34 **ATOM** 1920 CA PHE 405 60.250 40.221 30.198 1.00 39.33 **ATOM** 1921 CB PHE 405 61.620 40.840 29.913 1.00 33.87 405 **ATOM** 1922 CG PHE 62.107 40.609 28.509 1.00 32.17 **ATOM** 1923 CD1 PHE 405 62.355 41.683 27.660 1.00 31.34 **ATOM** 1924 CD2 PHE 405 62.315 39.317 28.032 1.00 31.98 405 **ATOM** 1925 CE1 PHE 62.801 41.476 26.352 1.00 30.79 **ATOM** 1926 CE2 PHE 405 62.759 39.099 26.730 1.00 26.06 63.004 40.182 25.889 1.00 27.98 **ATOM** 1927 CZ PHE 405 **ATOM** 1928 C PHE 405 59.905 40.322 31.682 1.00 42.64 1929 O **ATOM** PHE 405 60.785 40.188 32.534 1.00 45.10 **ATOM** 1930 N GLU 406 58.630 40.536 31.988 1.00 48.95 **ATOM** 1931 CA GLU 406 58.181 40.641 33.373 1.00 56.93

ATON (1000 OD OTT 404	# C 0 0 11 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM ATOM	1932 CB GLU 406	56.820 41.324 33.432 1.00 56.94
ATOM	1933 C GLU 406 1934 O GLU 406	58.116 39.263 34.040 1.00 61.92
		57.988 38.256 33.308 1.00 67.61
ATOM	1 O1 HOH 501	67.588 36.828 11.225 1.00 27.32
ATOM	2 O1 HOH 502	68.647 41.203 12.940 1.00 39.54
ATOM	3 O1- HOH 503	64.072 40.115 12.407 1.00 32.47
ATOM	4 O1 HOH 504	62.312 39.659 16.075 1.00 17.39
ATOM	5 O1 HOH 505	63.449 46.468 15.530 1.00 30.46
ATOM	6 O1 HOH 506	67.191 15.561 -0.279 1.00 35.96
ATOM	7 O1 HOH 507	67.100 11.855 0.295 1.00 20.00
ATOM	8 O1 HOH 508	61.004 15.510 0.047 1.00 20.00
ATOM	9 O1 HOH 509	59.851 10.761 6.050 1.00 20.00
ATOM	10 O1 HOH 510	57.553 11.824 10.360 1.00 44.63
ATOM	11 O1 HOH 511	54.101 13.545 8.720 1.00 20.00
ATOM	12 O1 HOH 512	55.923 15.916 12.205 1.00 29.31
ATOM	13 O1 HOH 513	50.900 19.934 8.193 1.00 20.00
ATOM	14 O1 HOH 514	50.474 22.912 7.942 1.00 45.34
ATOM	15 O1 HOH 515	49.737 20.631 11.530 1.00 20.00
ATOM	16 O1 HOH 516	50.829 25.467 13.330 1.00 20.00
ATOM	17 O1 HOH 517	53.818 25.833 10.682 1.00 42.12
ATOM	18 O1 HOH 518	52.591 31.216 7.313 1.00 35.55
ATOM	19 O1 HOH 519	58.510 31.667 2.158 1.00 20.00
ATOM	20 O1 HOH 520	58.235 36.751 2.232 1.00 20.00
ATOM	21 O1 HOH 521	62.484 37.992 5.537 1.00 20.00
ATOM	22 O1 HOH 522	68.184 36.969 5.889 1.00 50.08
ATOM	23 O1 HOH 523	66.889 33.781 8.584 1.00 20.00
ATOM	24 O1 HOH 524	67.217 30.836 3.085 1.00 34.44
ATOM	25 O1 HOH 525	64.336 28.325 3.098 1.00 20.00
ATOM	26 O1 HOH 526	67.667 26.625 1.519 1.00 20.00
ATOM	27 O1 HOH 527	76.757 22.883 5.467 1.00 36.94
ATOM	28 O1 HOH 528	72.250 17.936 6.950 1.00 36.00
ATOM	29 O1 HOH 529	71.760 14.791 8.058 1.00 40.18
ATOM	30 O1 HOH 530	72.884 14.751 11.484 1.00 41.44
ATOM	31 O1 HOH 531	69.235 12.986 11.709 1.00 39.38
ATOM	32 O1 HOH 532	69.402 12.036 14.891 1.00 40.68
ATOM	33 O1 HOH 533	64.560 10.910 15.076 1.00 20.00
ATOM	34 O1 HOH 534	63.169 10.413 11.722 1.00 20.00
ATOM	35 O1 HOH 535	66.042 11.455 11.077 1.00 41.05
ATOM	36 O1 HOH 536	76.285 12.458 10.677 1.00 20.00
ATOM	37 O1 HOH 537	81.094 22.520 13.435 1.00 48.70
ATOM	38 O1 HOH 538	80.505 25.457 14.849 1.00 46.30
ATOM	39 O1 HOH 539	77.669 21.932 18.119 1.00 43.79
ATOM	40 O1 HOH 540	77.187 28.903 21.137 1.00 40.22
ATOM	41 O1 HOH 541	76.420 30.760 23.658 1.00 29.63
ATOM	42 O1 HOH 542	83.028 32.743 20.922 1.00 38.14
ATOM	43 O1 HOH 543	82.842 43.133 17.983 1.00 39.36
ATOM	44 O1 HOH 544	77.484 34.040 9.664 1.00 36.37

ATOM	[45	5 0	1 НОН	545	75.904	4 32.986	5 12.256	1.00 34.93
ATOM	I 46	5 O	1 HOH	546	74.185	29.689	9.761	
ATOM	[47	7 0:	HOH I	547	64.936	5 20.644	23.365	1.00 36.83
ATOM	[48	O 2	l HOH	548	61.750	22.313	25.288	1.00 34.81
ATOM	49	01	HOH	549	59.544	21.463	26.162	
ATOM	50	O 1	HOH	550	62.300	27.528	24.386	1.00 35.89
ATOM	51	O1	HOH	551	58.228	3 29.424	24.603	
ATOM	52	01	HOH	552	57.368	32.196	30.527	1.00 45.27
ATOM	53	01	HOH	553	62.063	36.304	30.245	1.00 42.26
ATOM	54	O 1	HOH	554	64.722	36.725	28.906	1.00 24.66
ATOM	55	O 1	HOH	555	62.207	35.851	26.642	1.00 30.36
ATOM	56	O 1	HOH	556	63.608	33.715	25.707	1.00 42.74
ATOM	57	01	HOH	557	62.979	38.422	32.977	1.00 49.93
ATOM	58	O 1	HOH	558	66.911	33.364	34.901	1.00 50.02
ATOM	59	01	HOH	559	72.608	29.636	31.674	1.00 37.60
ATOM	60	01	HOH	560	76.967	40.633	32.514	1.00 44.81
ATOM	61	O 1	HOH	561	73.613	41.817	36.847	1.00 31.79
ATOM	62	01	HOH	562	75.773	46.227	30.514	1.00 29.06
ATOM	63	01	HOH	563	79.903	46.178	30.800	1.00 41.67
ATOM	64	01	HOH	564	69.746	51.175	33.564	1.00 20.00
ATOM	65	01	HOH	565	74.320	52.047	39.438	1.00 20.00
ATOM	66	01	HOH	566	65.900	53.647	27.404	1.00 40.45
ATOM	67	01	HOH	567	68.848	53.076	17.895	1.00 39.25
ATOM	68	01	HOH	568	63.507	48.672	13.581	1.00 43.77
ATOM	69	01	HOH	569	64.625	46.825	10.331	1.00 20.00
ATOM	70	01	HOH	570	55.882	41.431	11.148	1.00 20.00
ATOM	71	01	HOH	571	52.830	43.513	20.032	1.00 35.18
ATOM	72	01	HOH	572	56.990	49.485	24.052	1.00 37.30
ATOM	73	01	НОН	573	54.188	47.024	30.900	1.00 52.93
ATOM	74	01	HOH	574	57.823	44.590	34.025	1.00 53.64
ATOM	75	01	НОН	575	47.827	29.597	30.690	1.00 37.61
ATOM			НОН	576	53.030			1.00 45.06
ATOM	77	01	НОН	577	47.569			1.00 38.88
ATOM	78	01	НОН	578	47.232			1.00 20.00
ATOM	79		НОН	579				1.00 49.45
ATOM	80	01	HOH	580	52.831			1.00 20.00
ATOM	81	01	НОН	581		22.968		1.00 25.10
ATOM	82	01	HOH	582	77.238	52.503	8.906	1.00 47.05
END	2004	~ 1	D) (T)		<i>(5</i> , 220	10.006	10.640	1 00 00 50
ATOM			DMT	1				1.00 28.58
ATOM			DMT	1		43.263		1.00 29.26
ATOM			DMT	1	67.236			1.00 24.54
ATOM			DMT	1		44.313		1.00 28.48
ATOM	2008		DMT	1	68.003			1.00 28.76
ATOM	2009		DMT	1	68.654			1.00 28.16
ATOM			DMT	1	68.811			1.00 26.80
ATOM	2011	Ċδ	DMT	1	67.803	43.410	23.793	1.00 29.83

	0010	60 51 6	_				
ATOM	2012	C9 DMT	1	68.921	41.665	20.324	1.00 26.77
ATOM	2013	C10 DMT	1	67.464	42.358	24.989	1.00 28.60
ATOM	2014	C11 DMT	1	68.165	41.349	19.185	1.00 25.29
ATOM	2015	C12 DMT	1	68.059	42.281	23.675	1.00 26.74
ATOM	2016	C13 DMT	1	66.475	42.038	17.456	1.00 21.51
ATOM	2017	C14 DMT	1	68.916	45.478	26.380	1.00 21.05
ATOM	2018	C15 DMT	1	66.989	40.910	16.417	1.00 22.84
ATOM	2019	C16 DMT	1	68.090	46.870	26.009	1.00 19.41
ATOM	2020	C17 DMT	1	65.982	40.730	15.243	1.00 27.07
ATOM	2021	C18 DMT	1	70.279	46.131	26.085	1.00 16.03
ATOM	2022	C19 DMT	1	67.903	45.249	20.974	1.00 19.56
ATOM	2023	C20 DMT	1	69.853	40.599	20.901	1.00 4.52
ATOM	2024	N1 DMT	1	68.280	41.070	16.042	1.00 17.57
ATOM	2025	O1 DMT	. 1	67.209	43.465	27.087	1.00 25.94
ATOM	2026	O2 DMT	1	69.547	43.191	22.015	1.00 30.23
ATOM	2027	O3 DMT	1	66.449	40.778	14.118	1.00 29.45
ATOM	2028	O4 DMT	1	64.820	40.564	15.546	1.00 26.46
END							

APPENDIX 4

TR TRIAC.PDB

REMARK REMARK TR triac full length numbering REMARK Rfactor 0.236 Rfree 0.241 REMARK Resolution 25. 2.5 all reflections REMARK REMARK Three cacodylate-modified cysteines: REMARK Cys334, Cys380, Cys392 REMARK modeled as free arsenic atoms REMARK REMARK conserved polar HOH numbered as in TR t3.pdb REMARK rearrangements start 600 REMARK REMARK side chain of certain residues modeled as ALA due to poor density; REMARK however, residue name reflects true residue for clarity REMARK REMARK clone obtained from Murray et. al. REMARK deposited sequence confirmed, REMARK differing from that reported by Thompson et. al. REMARK in the following codons: REMARK 281 Thr - Ala REMARK 285 Lys - Glu REMARK identical to that reported by Mitsuhashi et. al. REMARK gb:RNTRAVI X07409 AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY, M.J.MACDONALD JRNL JRNL **AUTH 2 H.C.TOWLE** TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES JRNL FOR TWO TITL 2 DISTINCT THYROID HORMONE RECPTORS JRNL. JRNL REF **JBC** V. 263 25 1988 AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR JRNL **EXPRESSED** JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM JRNL REF **SCIENCE** V. 237 1987 AUTH T.MITSUHASHI, G.TENNYSON, V.NIKODEM JRNL JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY ALTERNATIVE JRNL TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE TRANSCRIPT **JRNL** REF NUC. ACIDS. RES. V. 16 12 1988 REMARK ATOM 1 CB ARG 157 9.880 -24.199 7.196 1.00 57.79

11.380 -24.411 7.340 1.00 57.79

21388546 189

2 CG ARG 157

ATOM

ATOM	3 CD ARG 157	11.960 -23.602 8.486 1.00 57.79
ATOM	4 NE ARG 157	11.492 -24.098 9.778 1.00 57.79
ATOM	5 CZ ARG 157	12.284 -24.379 10.809 1.00 57.79
ATOM	6 NH1 ARG 157	13.598 -24.212 10.714 1.00 57.79
ATOM	7 NH2 ARG 157	11.762 -24.854 11.932 1.00 57.79
ATOM	8 C ARG 157	7.774 -24.838 5.974 1.00 38.50
ATOM	9 O ARG 157	7.553 -24.416 4.840 1.00 57.79
ATOM	10 N ARG 157	9.929 -25.500 5.089 1.00 38.50
ATOM	11 CA ARG 157	9.183 -25.276 6.360 1.00 38.50
ATOM	12 N PRO 158	6.802 -24.951 6.895 1.00 23.08
ATOM	13 CD PRO 158	6.945 -25.424 8.282 1.00 28.38
ATOM	14 CA PRO 158	5.415 -24.562 6.617 1.00 23.08
ATOM	15 CB PRO 158	4.704 -24.824 7.948 1.00 28.38
ATOM	16 CG PRO 158	5.801 -24.735 8.966 1.00 28.38
ATOM	17 C PRO 158	5.210 -23.124 6.132 1.00 23.08
ATOM	18 O PRO 158	5.678 -22.167 6.753 1.00 28.38
ATOM	19 N GLU 159	4.504 -23.000 5.012 1.00 19.26
ATOM	20 CA GLU 159	4.191 -21.717 4.389 1.00 19.26
ATOM	21 CB GLU 159	4.022 -21.912
ATOM	22 CG GLU 159	5.317 -22.009 2.086 1.00 24.58
ATOM ATOM	23 CD GLU 159 24 OE1 GLU 159	5.849 -20.651 1.659 1.00 24.58
ATOM	24 OE1 GLU 159 25 OE2 GLU 159	5.034 -19.722
ATOM	26 C GLU 159	
ATOM	27 O GLU 159	2.879 -21.193 4.968 1.00 19.26 2.152 -21.931 5.636 1.00 24.58
ATOM	28 N PRO 160	2.579 -19.899 4.765 1.00 17.44
ATOM	29 CD PRO 160	3.442 -18.817 4.259 1.00 13.94
ATOM	30 CA PRO 160	1.323 -19.360 5.299 1.00 17.44
ATOM	31 CB PRO 160	1.414 -17.872 4.956 1.00 13.94
ATOM	32 CG PRO 160	2.880 -17.604 4.952 1.00 13.94
ATOM	33 C PRO 160	0.098 -20.006 4.639 1.00 17.44
ATOM	34 O PRO 160	0.067 -20.207 3.423 1.00 13.94
ATOM	35 N THR 161	-0.895 -20.352 5.450 1.00 17.00
ATOM	36 CA THR 161	-2.119 -20.957 4.941 1.00 17.00
ATOM	37 CB THR 161	-2.958 -21.587 6.086 1.00 20.43
ATOM	38 OG1 THR 161	-3.441 -20.557 6.959 1.00 20.43
ATOM	39 CG2 THR 161	-2.121 -22.576 6.888 1.00 20.43
ATOM	40 C THR 161	-2.929 -19.843 4.284 1.00 17.00
ATOM	41 O THR 161	-2.691 -18.660 4.547 1.00 20.43
ATOM	42 N PRO 162	-3.918 -20.200 3.449 1.00 12.94
ATOM	43 CD PRO 162	-4.311 -21.559 3.038 1.00 17.56
ATOM	44 CA PRO 162	-4.743 -19.190 2.780 1.00 12.94
ATOM	45 CB PRO 162	-5.846 -20.029 2.143 1.00 17.56
ATOM	46 CG PRO 162	-5.147 -21.303 1.816 1.00 17.56
ATOM	47 C PRO 162	-5.317 -18.171 3.763 1.00 12.94
ATOM	48 O PRO 162	-5.305 -16.964 3.503 1.00 17.56
ATOM	49 N GLU 163	-5.790 -18.668 4.903 1.00 19.45

ATOM	-50 CA GLU 163	-6.374 -17.828 5.943 1.00 19.45
ATOM	51 CB GLU 163	-6.994 -18.690 7.047 1.00 49.96
ATOM	52 CG GLU 163	-8.178 -19.558 6.606 1.00 49.96
ATOM	53 CD GLU 163	-7.782 -20.720 5.697 1.00 49.96
ATOM	54 OE1 GLU 163	-6.735 -21.361 5.951 1.00 49.96
ATOM	55 OE2 GLU 163	-8.527 -20.999 4.731 1.00 49.96
ATOM	56 C GLU 163	-5.330 -16.897 6.548 1.00 19.45
ATOM	57 O GLU 163	-5.614 -15.731 6.832 1.00 49.96
ATOM	58 N GLU 164	-4.120 -17.417 6.734 1.00 22.03
ATOM	59 CA GLU 164	-3.033 -16.634 7.305 1.00 22.03
ATOM	60 CB GLU 164	-1.875 -17.541 7.725 1.00 17.15
ATOM	61 CG GLU 164	-2.198 -18.414 8.937 1.00 17.15
ATOM	62 CD GLU 164	-1.114 -19.434 9.249 1.00 17.15
ATOM	63 OE1 GLU 164	-0.283 -19.710 8.361 1.00 17.15
ATOM	64 OE2 GLU 164	-1.099 -19.968 10.379 1.00 17.15
ATOM	65 C GLU 164	-2.559 -15.542 6.354 1.00 22.03
ATOM	66 O GLU 164	-2.160 -14.470 6.802 1.00 17.15
ATOM	67 N TRP 165	-2.607 -15.805 5.048 1.00 10.72
ATOM	68 CA TRP 165	-2.205 -14.803 4.063 1.00 10.72
ATOM -	69 CB TRP 165	-2.223 -15.377 2.644 1.00 2.00
ATOM	70 CG TRP 165	-0.928 -16.003 2.227 1.00 2.00
ATOM	71 CD2 TRP 165	0.350 -15.358 2.131 1.00 2.00
ATOM	72 CE2 TRP 165	1.275 -16.326
ATOM	73 CE3 TRP 165	0.804 -14.054 2.379 1.00 2.00
ATOM	74 CD1 TRP 165	-0.731 -17.298 1.848 1.00 2.00
ATOM	75 NE1 TRP 165	0.587 -17.500 1.521 1.00 2.00
ATOM	76 CZ2 TRP 165	2.627 -16.036 1.479 1.00 2.00
ATOM	77 CZ3 TRP 165	2.152 -13.764 2.174 1.00 2.00
ATOM	78 CH2 TRP 165	3.046 -14.754 1.729 1.00 2.00
ATOM	79 C TRP 165	-3.137 -13.601 4.149 1.00 10.72
ATOM	80 O TRP 165	-2.717 -12.463 3.925 1.00 2.00
ATOM	81 N ASP 166	-4.408 -13.861 4.441 1.00 14.80
ATOM	82 CA ASP 166	-5.397 -12.796 4.580 1.00 14.80
ATOM	83 CB ASP 166	-6.812 -13.370 4.698 1.00 28.74
ATOM	84 CG ASP 166	-7.298 -13.999
ATOM ATOM	85 OD1 ASP 166	-6.909 -13.511
	86 OD2 ASP 166	-8.071 -14.978
ATOM	87 C ASP 166	-5.063 -11.981 5.819 1.00 14.80
ATOM ATOM	88 O ASP 166 89 N LEU 167	-5.056 -10.749 5.775 1.00 28.74
ATOM		-4.745 -12.682 6.906 1.00 11.01
ATOM	90 CA LEU 167 91 CB LEU 167	-4.383 -12.044 8.166 1.00 11.01 -4.036 -13.103 9.214 1.00 31.53
ATOM	92 CG LEU 167	
ATOM	92 CG LEU 167 93 CD1 LEU 167	-4.672 -12.975 10.601 1.00 31.53 -3.806 -13.709 11.619 1.00 31.53
ATOM	94 CD2 LEU 167	
ATOM	95 C LEU 167	-4.820 -11.507 10.989 1.00 31.53 -3.161 -11.159 7.933 1.00 11.01
ATOM	96 O LEU 167	-3.120 -10.006 8.367 1.00 31.53
VIOM	70 O LEU 10/	-3.120 -10.000 0.307 1.00 31.33

ATOM · 97 N ILE 168 -2.180 -11.714 7.228 1.00 13.18 **ATOM** 98 CA ILE 168 -0.937 -11.027 6.900 1.00 13.18 **ATOM** 99 CB ILE 168 0.015 -11.968 6.113 1.00 18.30 **ATOM** 100 CG2 ILE 168 1.118 -11.182 5.414 1.00 18.30 **ATOM** 101 CG1 ILE 168 0.604 -13.013 7.063 1.00 18.30 **ATOM** 102 CD1 ILE 168 1.379 -14.111 6.373 1.00 18.30 **ATOM** 103 C ILE 168 -1.185 -9.747 6.107 1.00 13.18 ILE **ATOM** 104 O 168 -0.637 -8.697 6.437 1.00 18.30 **ATOM** 105 N HIS 169 -2.032 -9.831 5.084 1.00 12.99 **ATOM 106 CA HIS** 169 -2.342 -8.674 4.245 1.00 12.99 **ATOM** 107 CB HIS 169 -3.218 -9.087 3.062 1.00 13.09 **ATOM** 108 CG HIS 169 -2.553 -10.045 2.126 1.00 13.09 **ATOM** 109 CD2 HIS 169 -1.247 -10.223 1.811 1.00 13.09 **ATOM** 110 ND1 HIS 169 -3.249 -11.000 1.416 1.00 13.09 **ATOM** -2.403 -11.728 111 CE1 HIS 169 0.710 1.00 13.09 **ATOM** 112 NE2 HIS 169 -1.181 -11.277 0.936 1.00 13.09 **ATOM** HIS 113 C 169 -3.017 -7.550 5.017 1.00 12.99 **ATOM** 114 O HIS 169 -2.680 -6.377 4.839 1.00 13.09 **ATOM** 115 N VAL 170 -3.978 -7.909 5.862 1.00 13.36 **ATOM** 116 CA VAL 170 -4.696 -6.926 6.664 1.00 13.36 **ATOM** 117 CB VAL 170 -5.863 -7.572 7.443 1.00 20.12 **ATOM** 118 CG1 VAL 170 -6.541 -6.540 8.340 1.00 20.12 **ATOM** 119 CG2 VAL 170 -6.869 -8.165 6.471 1.00 20.12 **ATOM** 120 C -3.741 -6.246 VAL 170 7.639 1.00 13.36 **ATOM** 121 O VAL -3.728 -5.019 170 7.744 1.00 20.12 **ATOM** 122 N ALA 171 -2.920 -7.043 8.320 1.00 11.04 **ATOM** 123 CA ALA 171 -1.953 -6.515 9.277 1.00 11.04 124 CB ALA **ATOM** 171 -1.249 -7.653 10.005 1.00 13.43 **ATOM** 125 C ALA 171 -0.931 -5.613 8.588 1.00 11.04 **ATOM** 126 O **ALA** 171 -0.658 -4.507 9.058 1.00 13.43 127 N **ATOM** THR 172 -0.382 -6.076 7.469 1.00 12.51 **ATOM 128 CA THR** 172 0.606 -5.301 6.723 1.00 12.51 **ATOM** 129 CB THR 172 1.062 -6.032 5.445 1.00 14.17 **ATOM** 130 OG1 THR 172 1.548 -7.338 5.782 1.00 14.17 **ATOM** 131 CG2 THR 2.175 -5.255 4.756 1.00 14.17 172 **ATOM** 132 C THR 172 0.045 -3.936 6.337 1.00 12.51 **ATOM** 133 O THR 172 0.701 -2.910 6.537 1.00 14.17 **ATOM** 134 N GLU 173 -1.178 -3.921 5.815 1.00 17.79 135 CA GLU **ATOM** 173 -1.818 -2.675 5.421 1.00 17.79 **ATOM** 136 CB GLU 173 -3.130 -2.946 4.682 1.00 49.44 **ATOM** 137 CG GLU 173 -3.823 -1.679 4.171 1.00 49.44 **ATOM** 138 CD GLU 173 -2.930 -0.835 3.266 1.00 49.44 **ATOM** 139 OE1 GLU 173 -2.075 -1.408 2.552 1.00 49.44 **ATOM** 140 OE2 GLU 173 -3.085 0.404 3.269 1.00 49.44 **ATOM** 141 C GLU 173 -2.072 -1.780 6.628 1.00 17.79 **ATOM** 142 O **GLU** 173 -1.854 -0.568 6.557 1.00 49.44 **ATOM** 143 N **ALA** 174 -2.525 -2.375 7.731 1.00 13.12

ATOM 144 CA ALA 174 -2.798 -1.631 8.957 1.00 13.12 **ATOM** 145 CB ALA 174 -3.226 -2.576 10.068 1.00 17.51 **ATOM** 146 C ALA 174 -1.556 -0.856 9.375 1.00 13.12 **ATOM** 147 O ALA 174 -1.634 0.319 9.735 1.00 17.51 **ATOM** 148 N HIS 175 -0.409 -1.521 9.317 1.00 12.20 **ATOM** 149 CA HIS 175 0.851 -0.895 9.679 1.00 12.20 **ATOM** 150 CB HIS 175 1.944 -1.949 9.886 1.00 17.52 **ATOM** 151 CG HIS 175 3.302 -1.365 10.136 1.00 17.52 **ATOM** 152 CD2 HIS 175 3.733 -0.468 11.055 1.00 17.52 **ATOM** 153 ND1 HIS 175 4.400 -1.679 9.364 1.00 17.52 **ATOM** 154 CE1 HIS 175 5.447 -0.999 9.793 1.00 17.52 **ATOM** 155 NE2 HIS 175 5.070 -0.258 10.818 1.00 17.52 **ATOM** 156 C HIS 175 1.311 0.133 8.654 1.00 12.20 **ATOM** 157 O HIS 175 1.700 1.240 9.024 1.00 17.52 **ATOM** 158 N **ARG** 176 1.291 -0.233 7.375 1.00 12.54 **ATOM 159 CA ARG** 176 1.735 0.677 6.328 1.00 12.54 **ATOM** 160 CB ARG 176 1.662 0.017 4.950 1.00 50.41 **ATOM** 161 CG ARG 176 2.683 -1.088 4.730 1.00 50.41 **ATOM** 162 CD ARG 176 2.666 -1.565 3.299 1.00 50.41 **ATOM** 163 NE ARG 176 3.682 -2.571 2.989 1.00 50.41 **ATOM** 164 CZ ARG 176 3.577 -3.472 2.012 1.00 50.41 **ATOM** 165 NH1 ARG 176 2.496 -3.513 1.236 1.00 50.41 **ATOM** 166 NH2 ARG 176 4.536 -4.376 1.841 1.00 50.41 **ATOM** 167 C **ARG** 176 0.972 1.988 6.306 1.00 12.54 **ATOM ARG** 168 O 176 1.561 3.040 6.087 1.00 50.41 **ATOM** 169 N SER 177 -0.326 1.935 6.581 1.00 24.74 **ATOM** 170 CA SER -1.147 177 3.145 6.584 1.00 24.74 **ATOM** 171 CB SER 177 -2.6222.792 6.414 1.00 21.56 **ATOM** 172 OG SER 177 -3.069 1.913 7.436 1.00 21.56 **ATOM** 173 C SER 177 -0.960 4.013 7.832 1.00 24.74 **ATOM** 174 O SER 177 -1.401 5.159 7.863 1.00 21.56 **ATOM** 175 N THR 178 -0.347 3.453 8.870 1.00 17.96 176 CA THR **ATOM** 178 -0.104 4.181 10.115 1.00 17.96 **ATOM** 177 CB THR 178 -0.736 3.440 11.323 1.00 19.76 **ATOM** 178 OG1 THR 178 -0.265 2.091 11.361 1.00 19.76 **ATOM** 178 179 CG2 THR -2.253 3.443 11.211 1.00 19.76 **ATOM** 1.376 4.395 10.382 1.00 17.96 180 C THR 178 **ATOM** 181 O THR 178 1.760 4.880 11.445 1.00 19.76 182 N **ATOM ASN** 179 2.207 4.024 9.417 1.00 25.88 **ATOM 183 CA ASN** 179 3.654 4.180 9.546 1.00 25.88 ATOM -184 CB ASN 179 4.362 2.974 8.943 1.00 44.29 **ATOM 185 CG ASN** 179 5.817 2.871 9.368 1.00 44.29 **ATOM** 186 OD1 ASN 179 6.129 2.768 10.564 1.00 44.29 **ATOM** 187 ND2 ASN 179 6.719 2.830 8.391 1.00 44.29 **ATOM** 179 188 C ASN 5.458 8.823 1.00 25.88 4.078 **ATOM** 189 O **ASN** 179 4.150 5.495 7.590 1.00 44.29 **ATOM** 190 N **ALA** 180 4.332 6.502 9.604 1.00 45.20

ATOM	191 CA ALA 180	4.740 7.818 9.126 1.00 45.20
ATOM	192 CB ALA 180	5.026 8.743 10.313 1.00 36.14
ATOM	193 C ALA 180	5.931 7.808 8.170 1.00 45.20
ATOM	194 O ALA 180	6.918 7.097 8.372 1.00 36.14
ATOM	195 N ALA 181	5.784 8.552 7.080 1.00 44.05
ATOM	196 CA ALA 181	6.834 8.661 6.072 1.00 44.05
ATOM	197 CB ALA 181	8.170 9.116 6.722 1.00 50.21
ATOM	198 C ALA 181	7.069 7.427 5.196 1.00 44.05
ATOM	199 O ALA 181	7.663 7.550 4.118 1.00 50.21
ATOM	200 N GLY 182	6.567 6.268 5.622 1.00 39.06
ATOM	201 CA GLY 182	6.756 5.040 4.867 1.00 39.06
ATOM	202 C GLY 182	8.202 4.769 4.482 1.00 39.06
ATOM	203 O GLY 182	9.096 4.785 5.334 1.00 48.58
ATOM	204 N SER 183	8.438 4.564 3.189 1.00 64.55
ATOM	205 CA SER 183	9.781 4.270 2.693 1.00 64.55
ATOM	206 CB SER 183	9.690 3.402 1.430 1.00 67.68
ATOM	207 OG SER 183	8.822 3.978 0.467 1.00 67.68
ATOM	208 C SER 183	10.643 5.510 2.437 1.00 64.55
ATOM	209 O SER 183	11.839 5.407 2.158 1.00 67.68
ATOM	210 N HIS 184	10.035 6.683 2.579 1.00 52.73
ATOM	211 CA HIS 184	10.725 7.953 2.352 1.00 52.73
ATOM	212 CB HIS 184	9.772 8.955 1.698 1.00 44.77
ATOM	213 C HIS 184	11.364 8.582 3.595 1.00 52.73
ATOM	214 O HIS 184	11.837 9.722 3.540 1.00 44.77
ATOM	215 N TRP 185	11.420 7.842 4.699 1.00 54.14
ATOM	216 CA TRP 185	11.977 8.389 5.940 1.00 54.14
ATOM	217 CB TRP 185	11.813 7.395 7.104 1.00 40.24
ATOM	218 CG TRP 185	12.605 6.123 6.991 1.00 40.24
ATOM	219 CD2 TRP 185	13.894 5.873 7.551 1.00 40.24
ATOM	220 CE2 TRP 185	14.245 4.543 7.221 1.00 40.24
ATOM	221 CE3 TRP 185	14.791 6.641 8.300 1.00 40.24
ATOM	222 CD1 TRP 185	12.227 4.973 6.359 1.00 40.24
ATOM	223 NE1 TRP 185	13.210 4.015 6.496 1.00 40.24
ATOM	224 CZ2 TRP 185	15.461 3.968 7.619 1.00 40.24
ATOM	225 CZ3 TRP 185	15.996 6.073 8.696 1.00 40.24
ATOM ATOM	226 CH2 TRP 185 227 C TRP 185	16.319 4.747 8.353 1.00 40.24
ATOM		13.432 8.870 5.819 1.00 54.14
ATOM	228 O TRP 185	13.759 10.008 6.168 1.00 40.24
ATOM	229 N LYS 186 230 CA LYS 186	14.277 8.032 5.232 1.00 43.72
		15.694 8.329 5.035 1.00 43.72
ATOM	231 CB LYS 186	16.353 7.168 4.282 1.00 64.14
ATOM	232 CG LYS 186	17.830 7.355 3.945 1.00 64.14
ATOM	233 CD LYS 186	18.758 7.175 5.139 1.00 64.14
ATOM	234 CE LYS 186	20.195 7.060 4.652 1.00 64.14
ATOM	235 NZ LYS 186	20.348 5.838 3.805 1.00 64.14
ATOM	236 C LYS 186	15.900 9.634 4.263 1.00 43.72
ATOM	237 O LYS 186	16.948 10.256 4.366 1.00 64.14

. ATOM	238 N GLN 187	14.892 10.032 3.491 1.00 58.06
ATOM	239 CA GLN 187	14.958 11.244 2.682 1.00 58.06
ATOM	240 CB GLN 187	14.288 10.997 1.321 1.00 74.68
ATOM	241 CG GLN 187	14.639 9.662 0.667 1.00 74.68
ATOM	242 CD GLN 187	16.133 9.397 0.607 1.00 74.68
ATOM	243 OE1 GLN 187	16.926 10.312 0.381 1.00 74.68
ATOM	244 NE2 GLN 187	16.528 8.156 0.855 1.00 74.68
ATOM	245 C GLN 187	14.322 12.466 3.342 1.00 58.06
ATOM	246 O GLN 187	14.897 13.551 3.358 1.00 74.68
ATOM	247 N ARG 188	13.117 12.280 3.866 1.00 54.11
ATOM	248 CA ARG 188	12.363 13.360 4.505 1.00 54.11
ATOM	249 CB ARG 188	10.889 13.115 4.334 1.00 53.33
ATOM	250 C ARG 188	12.654 13.626 5.977 1.00 54.11
ATOM	251 O ARG 188	11.879 14.298 6.659 1.00 53.33
ATOM	252 N ARG 189	13.754 13.090 6.473 1.00 39.52
ATOM	253 CA ARG 189	14.089 13.271 7.875 1.00 39.52
ATOM	254 CB ARG 189	14.594 11.959 8.482 1.00 60.85
ATOM	255 CG ARG 189	15.969 11.555 7.991 1.00 60.85
ATOM	256 CD ARG 189	16.442 10.298 8.693 1.00 60.85
ATOM	257 NE ARG 189	17.833 9.963 8.385 1.00 60.85
ATOM	258 CZ ARG 189	18.627 9.261 9.190 1.00 60.85
ATOM	259 NH1 ARG 189	18.178 8.805 10.356 1.00 60.85
ATOM	260 NH2 ARG 189	19.882 9.021 8.841 1.00 60.85
ATOM	261 C ARG 189	15.109 14.378 8.109 1.00 39.52
ATOM	262 O ARG 189	16.037 14.565 7.320 1.00 60.85
ATOM	263 N LYS 190	14.934 15.100 9.212 1.00 44.13
ATOM	264 CA LYS 190	15.834 16.183 9.586 1.00 44.13
ATOM	265 CB LYS 190	15.068 17.500 9.680 1.00 45.33
ATOM	266 C LYS 190	16.472 15.846 10.928 1.00 44.13
ATOM	267 O LYS 190	15.827 15.272 11.805 1.00 45.33
ATOM	268 N PHE 191	17.748 16.184 11.067 1.00 35.64
ATOM	269 CA PHE 191	18.489 15.928 12.291 1.00 35.64
ATOM	270 CB PHE 191	19.993 16.008 12.025 1.00 53.94
ATOM ATOM	271 CG PHE 191 272 CD1 PHE 191	20.550 14.827 11.286 1.00 53.94
ATOM	272 CD1 PHE 191 273 CD2 PHE 191	20.209 14.596 9.958 1.00 53.94
ATOM		21.430 13.949 11.915 1.00 53.94
ATOM		20.735 13.510 9.265 1.00 53.94
ATOM		21.964 12.859 11.230 1.00 53.94
ATOM	276 CZ PHE 191 277 C PHE 191	21.615 12.639 9.900 1.00 53.94 18.135 16.928 13.384 1.00 35.64
ATOM	278 O PHE 191	
ATOM	279 N LEU 192	17.997 18.127 13.120 1.00 53.94
ATOM		17.978 16.439 14.610 1.00 44.53
ATOM		17.683 17.315 15.736 1.00 44.53
ATOM		17.326 16.493 16.980 1.00 22.94
ATOM		16.931 17.259 18.246 1.00 22.94
ATOM	283 CD1 LEU 192 284 CD2 LEU 192	15.568 17.906 18.064 1.00 22.94
VIOM	284 CD2 LEU 192	16.909 16.308 19.427 1.00 22.94

ATOM ²⁸⁵ C LEU 192 18.974 18.101 15.980 1.00 44.53 **ATOM** 286 O LEU 192 20.049 17.507 16.129 1.00 22.94 **ATOM** 287 N **PRO** 193 18.895 19.444 15.977 1.00 34.26 **ATOM** 288 CD PRO 193 17.670 20.241 15.781 1.00 46.23 **ATOM** 289 CA PRO 193 20.058 20.311 16.198 1.00 34.26 290 CB PRO **ATOM** 193 19.417 21.670 16.465 1.00 46.23 **ATOM** 291 CG PRO 193 18.213 21.641 15.579 1.00 46.23 **ATOM** 292 C **PRO** 193 20.917 19.844 17.372 1.00 34.26 **ATOM** 293 O **PRO** 193 20.413 19.614 18.471 1.00 46.23 **ATOM** 294 N **ASP** 194 22.217 19.716 17.125 1.00 42.67 **ATOM** 295 CA ASP 194 23.174 19.254 18.128 1.00 42.67 **ATOM** 296 CB ASP 194 24.583 19.226 17.536 1.00 68.50 **ATOM** 297 CG ASP 194 24.731 18.185 16.450 1.00 68.50 **ATOM** 298 OD1 ASP 194 25.066 17.027 16.782 1.00 68.50 **ATOM** 299 OD2 ASP 194 24.498 18.518 15.269 1.00 68.50 **ATOM** 300 C **ASP** 194 23.187 20.003 19.457 1.00 42.67 **ATOM** 301 O **ASP** 194 23.545 19.432 20.486 1.00 68.50 **ATOM** 302 N ASP 195 22.817 21.280 19.438 1.00 47.52 **ATOM** 303 CA ASP 195 22.793 22.070 20.666 1.00 47.52 304 CB ASP **ATOM** 195 22.586 23.559 20.351 1.00 85.02 **ATOM** 305 CG ASP 195 21.327 23.824 19.537 1.00 85.02 **ATOM** 306 OD1 ASP 195 20.291 24.188 20.138 1.00 85.02 **ATOM** 307 OD2 ASP 195 21.377 23.683 18.294 1.00 85.02 **ATOM** 308 C **ASP** 195 21.715 21.561 21.627 1.00 47.52 **ASP** 195 **ATOM** 309 O 21.762 21.826 22.831 1.00 85.02 **ATOM** 310 N ILE 196 20.760 20.810 21.089 1.00 44.54 **ATOM** 311 CA ILE 196 19.663 20.259 21.875 1.00 44.54 312 CB ILE **ATOM** 196 18.379 20.137 21.023 1.00 39.66 **ATOM** 313 CG2 ILE 196 17.223 19.627 21.874 1.00 39.66 **ATOM** 314 CG1 ILE 196 18.031 21.496 20.407 1.00 39.66 **ATOM** 315 CD1 ILE 196 16.816 21.475 19.503 1.00 39.66 **ATOM** 316 C ILE 196 20.030 18.882 22.420 1.00 44.54 **ATOM** 317 O ILE 196 20.582 18.046 21.705 1.00 39.66 **ATOM** 318 N GLY 197 19.714 18.652 23.690 1.00 42.85 **ATOM** 319 CA GLY 197 20.006 17.372 24.307 1.00 42.85 **ATOM** 320 C GLY 197 21.371 17.285 24.956 1.00 42.85 **ATOM** 321 O GLY 197 21.815 16.198 25.318 1.00 40.22 **ATOM** 322 N GLN 198 22.029 18.425 25.137 1.00 53.07 **ATOM 323 CA GLN** 198 23.351 18.444 25.754 1.00 53.07 **ATOM** 324 CB GLN 198 24.357 19.103 24.810 1.00 44.23 **ATOM** 325 C GLN 198 23.344 19.153 27.110 1.00 53.07 **GLN** 198 24.396 19.545 27.616 1.00 44.23 **ATOM** 326 O **ATOM** 327 N SER 199 22.170 19.244 27.729 1.00 35.30 **ATOM 328 CA SER** 199 22.037 19.918 29.019 1.00 35.30 **ATOM 329 CB SER** 199 21.472 21.328 28.806 1.00 58.72 **ATOM** 330 OG SER 199 22.093 21.971 27.704 1.00 58.72 **ATOM** 331 C SER 199 21.168 19.169 30.036 1.00 35.30

ATOM	332 O SER 199	20.135 19.681 30.482 1.00 58.72
ATOM	333 N PRO 200	21.544 17.928 30.387 1.00 34.70
ATOM	334 CD PRO 200	22.656 17.108 29.872 1.00 38.71
ATOM	335 CA PRO 200	20.740 17.184 31.362 1.00 34.70
ATOM	336 CB PRO 200	21.311 15.769 31.266 1.00 38.71
ATOM	337 CG PRO 200	22.737 15.992 30.878 1.00 38.71
ATOM	338 C PRO 200	20.923 17.784 32.759 1.00 34.70
ATOM	339 O PRO 200	22.006 17.692 33.341 1.00 38.71
ATOM	340 N ILE 201	19.876 18.413 33.286 1.00 42.94
ATOM	341 CA ILE 201	19.961 19.041 34.604 1.00 42.94
ATOM	342 CB ILE 201	20.059 20.582 34.491 1.00 51.32
ATOM	343 CG2 ILE 201	21.468 20.991 34.078 1.00 51.32
ATOM	344 CG1 ILE 201	19.009 21.111 33.510 1.00 51.32
ATOM	345 CD1 ILE 201	19.169 22.582 33.164 1.00 51.32
ATOM	346 C ILE 201	18.871 18.676 35.610 1.00 42.94
ATOM	347 O ILE 201	19.049 18.875 36.814 1.00 51.32
ATOM	348 N VAL 202	17.737 18.172 35.133 1.00 50.33
ATOM	349 CA VAL 202	16.661 17.787 36.043 1.00 50.33
ATOM ATOM	350 CB VAL 202 351 CG1 VAL 202	15.296 17.722 35.326 1.00 36.59
ATOM	351 CG1 VAL 202 352 CG2 VAL 202	14.202 17.311 36.304 1.00 36.59
ATOM	353 C VAL 202	14.968 19.074 34.714 1.00 36.59 17.007 16.435 36.665 1.00 50.33
ATOM	354 O VAL 202	17.335 15.481 35.955 1.00 36.59
ATOM	355 N SER 203	16.960 16.375 37.991 1.00 49.46
ATOM	356 CA SER 203	17.289 15.166 38.736 1.00 49.46
ATOM	357 CB SER 203	17.298 15.467 40.241 1.00 64.20
ATOM	358 OG SER 203	17.673 14.330 41.003 1.00 64.20
ATOM	359 C SER 203	16.356 13.992 38.463 1.00 49.46
ATOM	360 O SER 203	15.147 14.166 38.310 1.00 64.20
ATOM	361 N MET 204	16.944 12.800 38.419 1.00 41.99
ATOM	362 CA MET 204	16.223 11.551 38.205 1.00 41.99
ATOM	363 CB MET 204	16.320 11.096 36.746 1.00 48.64
ATOM	364 CG MET 204	15.470 11.895 35.771 1.00 48.64
ATOM	365 SD MET 204	13.702 11.783 36.114 1.00 48.64
ATOM	366 CE MET 204	13.284 10.257 35.264 1.00 48.64
ATOM	367 C MET 204	16.900 10.528 39.109 1.00 41.99
ATOM	368 O MET 204	18.127 10.417 39.121 1.00 48.64
ATOM	369 N PRO 205	16.108 9.754 39.869 1.00 38.42
ATOM ATOM	370 CD PRO 205	14.633 9.815 39.866 1.00 52.20
ATOM	371 CA PRO 205 372 CB PRO 205	16.586 8.724 40.797 1.00 38.42
ATOM	372 CB PRO 205 373 CG PRO 205	15.334 7.888 41.041 1.00 52.20
ATOM	374 C PRO 205	14.254 8.919 41.028 1.00 52.20
ATOM	375 O PRO 205	17.769 7.858 40.340 1.00 38.42 18.724 7.675 41.092 1.00 52.20
ATOM	376 N ASP 206	17.720 7.349 39.111 1.00 49.06
ATOM	377 CA ASP 206	18.791 6.490 38.601 1.00 49.06
ATOM	378 CB ASP 206	18.282 5.627 37.437 1.00 74.42
	2.0 CD ADI 200	10.202 3.02/ 37.43/ 1.00/4.42

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ATOM 379 CG ASP 206 17.690 6.450 36.305 1.00 74.42 **ATOM** 380 OD1 ASP 206 7.335 35.770 1.00 74.42 18.397 **ATOM** 381 OD2 ASP 206 16.516 6.199 35.948 1.00 74.42 ATOM 382 C ASP 206 20.106 7.177 38.214 1.00 49.06 **ATOM** 383 O **ASP** 206 21.069 6.506 37.838 1.00 74.42 **ATOM** 384 N. GLY 207 20.139 8.505 38.272 1.00 42.48 **ATOM** 385 CA GLY 207 21.355 9.225 37.928 1.00 42.48 **ATOM** 386 C GLY 207 21.330 9.965 36.601 1.00 42.48 **ATOM** 387 O **GLY** 207 21.890 11.058 36.494 1.00 42.50 **ATOM** 388 N **ASP** 208 20.725 9.365 35.581 1.00 46.70 **ATOM** 389 CA ASP 208 20.636 9.999 34.266 1.00 46.70 **ATOM** 390 CB ASP 208 20.162 8.994 33.212 1.00 61.56 **ATOM** 391 CG ASP 208 21.143 7.856 33.006 1.00 61.56 **ATOM** 392 OD1 ASP 208 20.723 6.684 33.122 1.00 61.56 22.330 8.134 32.724 1.00 61.56 **ATOM** 393 OD2 ASP 208 **ATOM** 394 C **ASP** 208 19.666 11.176 34.339 1.00 46.70 **ATOM** 395 O **ASP** 208 18.462 10.983 34.506 1.00 61.56 396 N LYS 209 **ATOM** 20.200 12.389 34.238 1.00 41.30 **ATOM** 397 CA LYS 209 19.389 13.602 34.308 1.00 41.30 **ATOM** 398 CB LYS 209 20.254 14.782 34.732 1.00 41.38 **ATOM** 399 C LYS 209 18.657 13.916 33.004 1.00 41.30 400 O **ATOM** LYS 209 19.052 13.458 31.930 1.00 41.38 **ATOM** 401 N VAL 210 17.603 14.723 33.109 1.00 43.36 **ATOM** 402 CA VAL 210 16.792 15.107 31.954 1.00 43.36 **ATOM** 403 CB VAL 210 15.275 15.014 32.282 1.00 30.23 **ATOM** 210 404 CG1 VAL 14.440 15.358 31.055 1.00 30.23 **ATOM** 405 CG2 VAL 210 14.923 13.624 32.782 1.00 30.23 **ATOM** 406 C VAL 210 17.088 16.522 31.442 1.00 43.36 **ATOM** 407 O VAL 210 17.395 17.430 32.221 1.00 30.23 **ATOM** 408 N **ASP** 211 17.004 16.685 30.125 1.00 27.49 **ATOM** 409 CA ASP 211 17.217 17.966 29.458 1.00 27.49 **ATOM** 410 CB ASP 211 18.073 17.765 28.198 1.00 30.75 **ATOM** 411 CG ASP 211 18.360 19.068 27.447 1.00 30.75 **ATOM** 412 OD1 ASP 211 19.473 19.196 26.900 1.00 30.75 **ATOM** 211 413 OD2 ASP 17.484 19.955 27.370 1.00 30.75 **ATOM** 414 C ASP 211 15.819 18.445 29.073 1.00 27.49 **ATOM** 415 O ASP 211 15.197 17.892 28.166 1.00 30.75 **ATOM** 416 N LEU 212 15.343 19.488 29.745 1.00 31.99 **ATOM** 417 CA LEU 212 14.013 20.042 29.492 1.00 31.99 418 CB LEU **ATOM** 212 13.778 21.274 30.369 1.00 35.19 **ATOM** 419 CG LEU 212 13.606 20.997 31.864 1.00 35.19 **ATOM** 420 CD1 LEU 212 13.621 22.298 32.652 1.00 35.19 **ATOM** 421 CD2 LEU 212 12.309 20.237 32.098 1.00 35.19 **ATOM** 422 C LEU 212 13.713 20.377 28.032 1.00 31.99 423 O **ATOM** LEU 212 12.625 20.083 27.539 1.00 35.19 **ATOM** 424 N GLU 213 14.672 20.981 27.338 1.00 28.70 **ATOM** 425 CA GLU 213 14.468 21.345 25.940 1.00 28.70

ATOM	426 CB GLU 213	15.623 22.209 25.428 1.00 62.21
ATOM	427 CG GLU 213	15.434 22.707 23.997 1.00 62.21
ATOM	428 CD GLU 213	16.651 23.440 23.446 1.00 62.21
ATOM	429 OE1 GLU 213	17.778 23.214 23.945 1.00 62.21
ATOM	430 OE2 GLU 213	16.478 24.237 22.498 1.00 62.21
ATOM	431 C GLU 213	14.317 20.104 25.067 1.00 28.70
ATOM	432 O GLU 213	13.403 20.024 24.247 1.00 62.21
ATOM	433 N ALA 214	15.201 19.130 25.262 1.00 28.17
ATOM	434 CA ALA 214	15.162 17.890 24.494 1.00 28.17
ATOM	435 CB ALA 214	16.330 16.998 24.872 1.00 42.74
ATOM	436 C ALA 214	13.844 17.176 24.759 1.00 28.17
ATOM	437 O ALA 214	13.174 16.726 23.829 1.00 42.74
ATOM	438 N PHE 215	13.468 17.104 26.032 1.00 21.66
ATOM	439 CA PHE 215	12.222 16.471 26.444 1.00 21.66
ATOM	440 CB PHE 215	12.033 16.628 27.958 1.00 28.76
ATOM	441 CG PHE 215	10.751 16.038 28.481 1.00 28.76
ATOM	442 CD1 PHE 215	10.675 14.689 28.815 1.00 28.76
ATOM	443 CD2 PHE 215	9.623 16.835 28.653 1.00 28.76
ATOM	444 CE1 PHE 215	9.493 14.143 29.315 1.00 28.76
ATOM	445 CE2 PHE 215	8.438 16.300 29.150 1.00 28.76
ATOM	446 CZ PHE 215	8.373 14.951 29.482 1.00 28.76
ATOM	447 C PHE 215	11.068 17.132 25.696 1.00 21.66
ATOM	448 O PHE 215	10.215 16.451 25.122 1.00 28.76
ATOM	449 N SER 216	11.073 18.462 25.680 1.00 28.03
ATOM	450 CA SER 216	10.043 19.242 25.007 1.00 28.03
ATOM	451 CB SER 216	10.349 20.734 25.146 1.00 33.85
ATOM	452 OG SER 216	9.300 21.529 24.624 1.00 33.85
ATOM	453 C SER 216	9.945 18.857 23.532 1.00 28.03
ATOM	454 O SER 216	8.852 18.613 23.019 1.00 33.85
ATOM	455 N GLU 217	11.092 18.761 22.868 1.00 28.84
ATOM	456 CA GLU 217	11.138 18.402 21.454 1.00 28.84
ATOM	457 CB GLU 217	12.581 18.420 20.943 1.00 47.68
ATOM	458 CG GLU 217	13.174 19.815 20.811 1.00 47.68
ATOM	459 CD GLU 217	12.405 20.684 19.829 1.00 47.68
ATOM	460 OE1 GLU 217	11.660 21.581 20.281 1.00 47.68
ATOM	461 OE2 GLU 217	12.542 20.465 18.606 1.00 47.68
ATOM	462 C GLU 217	10.505 17.044 21.179 1.00 28.84
ATOM	463 O GLU 217	9.751 16.886 20.217 1.00 47.68
ATOM	464 N PHE 218	10.799 16.071 22.036 1.00 21.49
ATOM	465 CA PHE 218	10.259 14.725 21.883 1.00 21.49
ATOM	466 CB PHE 218	11.020 13.746 22.781 1.00 24.12
ATOM	467 CG PHE 218	12.489 13.652 22.464 1.00 24.12
ATOM	468 CD1 PHE 218	13.431 13.554 23.481 1.00 24.12
ATOM	469 CD2 PHE 218	12.932 13.677 21.144 1.00 24.12
ATOM	470 CE1 PHE 218	14.793 13.484 23.187 1.00 24.12
ATOM	471 CE2 PHE 218	14.290 13.607 20.843 1.00 24.12
ATOM	472 CZ PHE 218	15.221 13.511 21.867 1.00 24.12

ATOM 473 C PHE 218 8.765 14.675 22.176 1.00 21.49 **ATOM** 474 O PHE 218 7.985 14.166 21.369 1.00 24.12 **ATOM** 475 N THR 219 8.358 15.227 23.312 1.00 20.07 476 CA THR **ATOM** 219 6.949 15.231 23.685 1.00 20.07 **ATOM** 477 CB THR 219 6.741 15.766 25.118 1.00 28.98 **ATOM** 478 OG1 THR 219 7.418 17.021 25.274 1.00 28.98 **ATOM** 479 CG2 THR 219 7.275 14.767 26.132 1.00 28.98 **ATOM** 480 C THR 219 6.080 16.011 22.696 1.00 20.07 **ATOM** 481 O THR 219 4.914 15.670 22.482 1.00 28.98 **ATOM** 482 N LYS 220 6.662 17.022 22.060 1.00 25.35 483 CA LYS **ATOM** 220 5.943 17.840 21.088 1.00 25.35 **ATOM** 484 CB LYS 220 6.842 18.965 20.577 1.00 29.07 **ATOM** 485 C LYS 220 5.414 17.015 19.916 1.00 25.35 **ATOM** 486 O LYS 220 4.376 17.343 19.339 1.00 29.07 487 N **ATOM** ILE 221 6.122 15.943 19.569 1.00 31.43 **ATOM 488 CA ILE** 221 5.708 15.089 18.458 1.00 31.43 **ATOM** 489 CB ILE 221 6.842 14.915 17.413 1.00 25.19 **ATOM** 490 CG2 ILE 221 7.240 16.264 16.838 1.00 25.19 **ATOM** 491 CG1 ILE 221 8.050 14.215 18.043 1.00 25.19 **ATOM** 492 CD1 ILE 221 9.113 13.799 17.044 1.00 25.19 **ATOM** 493 C ILE 221 5.240 13.700 18.892 1.00 31.43 **ATOM** 494 O ILE 221 4.930 12.857 18.046 1.00 25.19 ATOM 495 N ILE 222 5.129 13.474 20.198 1.00 24.41 **ATOM** 496 CA ILE 222 4.720 12.162 20.687 1.00 24.41 **ATOM** 497 CB ILE 222 5.189 11.916 22.147 1.00 27.10 **ATOM** 498 CG2 ILE 222 4.221 12.545 23.145 1.00 27.10 **ATOM** 499 CG1 ILE 222 5.302 10.410 22.400 1.00 27.10 **ATOM** 500 CD1 ILE 222 6.062 10.053 23.646 1.00 27.10 **ATOM** 501 C ILE 222 3.231 11.845 20.541 1.00 24.41 **ATOM** 502 O ILE 222 2.864 10.691 20.307 1.00 27.10 503 N **ATOM** THR 223 2.378 12.861 20.642 1.00 33.16 504 CA THR 223 ATOM 0.936 12.653 20.520 1.00 33.16 **ATOM** 505 CB THR 223 0.150 13.974 20.721 1.00 36.84 **ATOM** 506 OG1 THR 223 0.352 14.442 22.063 1.00 36.84 **ATOM** 507 CG2 THR 223 -1.346 13.764 20.484 1.00 36.84 **ATOM** 508 C 223 THR 0.536 11.954 19.212 1.00 33.16 **ATOM** 509 O THR 223 -0.156 10.932 19.242 1.00 36.84 **ATOM** 510 N PRO 224 0.968 12.482 18.048 1.00 18.75 **ATOM** 511 CD PRO 224 1.691 13.735 17.770 1.00 26.12 **ATOM** 512 CA PRO 224 0.590 11.805 16.802 1.00 18.75 **ATOM** 513 CB PRO 224 1.117 12.747 15.715 1.00 26.12 **ATOM** 2.221 13.497 16.386 1.00 26.12 514 CG PRO 224 **ATOM** 515 C PRO 224 1.200 10.402 16.701 1.00 18.75 **ATOM** 516 O PRO 224 0.606 9.502 16.101 1.00 26.12 2.368 10.213 17.312 1.00 12.19 **ATOM** 517 N ALA 225 **ATOM** 518 CA ALA 225 3.040 8.916 17.300 1.00 12.19 **ATOM** 519 CB ALA 225 4.415 9.021 17.943 1.00 20.39

ATOM	520 C ALA 225	2.187 7.881 18.030 1.00 12.19
ATOM	521 O ALA 225	1.998 6.764 17.545 1.00 20.39
ATOM	522 N ILE 226	1.645 8.271 19.179 1.00 14.61
ATOM	523 CA ILE 226	0.798 7.385 19.971 1.00 14.61
ATOM	524 CB ILE 226	0.450 8.025 21.332 1.00 16.10
ATOM	525 CG2 ILE 226	-0.508 7.132 22.108 1.00 16.10
ATOM	526 CG1 ILE 226	1.729 8.293 22.132 1.00 16.10
ATOM	527 CD1 ILE 226	1.509 9.113 23.387 1.00 16.10
ATOM	528 C ILE 226	-0.499 7.094 19.213 1.00 14.61
ATOM	529 O ILE 226	-0.986 5.961 19.200 1.00 16.10
ATOM	530 N THR 227	-1.042 8.123 18.569 1.00 15.93
ATOM	531 CA THR 227	-2.278 7.997 17.800 1.00 15.93
ATOM	532 CB THR 227	-2.706 9.360 17.207 1.00 22.37
ATOM	533 OG1 THR 227	-2.890 10.301 18.273 1.00 22.37
ATOM	534 CG2 THR 227	-4.014 9.232 16.434 1.00 22.37
ATOM	535 C THR 227	-2.149 6.964 16.680 1.00 15.93
ATOM	536 O THR 227	-3.091 6.217 16.402 1.00 22.37
ATOM	537 N ARG 228	-0.982 6.916 16.045 1.00 14.49
ATOM	538 CA ARG 228	-0.750 5.956 14.975 1.00 14.49
ATOM	539 CB ARG 228	0.602 6.188 14.307 1.00 33.87
ATOM	540 CG ARG 228	0.701 7.482 13.540 1.00 33.87
ATOM	541 CD ARG 228	2.053 7.572 12.868 1.00 33.87
ATOM	542 NE ARG 228	2.510 8.952 12.793 1.00 33.87
ATOM	543 CZ ARG 228	3.551 9.431 13.469 1.00 33.87
ATOM	544 NH1 ARG 228	4.256 8.634 14.270 1.00 33.87
ATOM	545 NH2 ARG 228	3.864 10.716 13.374 1.00 33.87
ATOM	546 C ARG 228	-0.813 4.531 15.516 1.00 14.49
ATOM	547 O ARG 228	-1.309 3.632 14.839 1.00 33.87
ATOM	548 N VAL 229	-0.313 4.327 16.735 1.00 14.80
ATOM	549 CA VAL 229	-0.333 3.002 17.352 1.00 14.80
ATOM	550 CB VAL 229	0.456 2.979 18.683 1.00 13.78
ATOM	551 CG1 VAL 229	0.339 1.612 19.350 1.00 13.78
ATOM ATOM	552 CG2 VAL 229 553 C VAL 229	1.915 3.312 18.430 1.00 13.78
ATOM	554 O VAL 229	-1.788 2.602 17.591 1.00 14.80 -2.185 1.465 17.323 1.00 13.78
ATOM	555 N VAL 230	-2.185 1.465 17.323 1.00 13.78 -2.588 3.561 18.047 1.00 9.33
ATOM	556 CA VAL 230	-4.005 3.327 18.292 1.00 9.33
ATOM	557 CB VAL 230	-4.679 4.564 18.909 1.00 16.07
	558 CG1 VAL 230	-6.168 4.319 19.076 1.00 16.07
ATOM	559 CG2 VAL 230	-4.038 4.896 20.253 1.00 16.07
ATOM	560 C VAL 230	-4.700 2.982 16.981 1.00 9.33
ATOM	561 O VAL 230	-5.504 2.049 16.929 1.00 16.07
ATOM	562 N ASP 231	-4.364 3.719 15.922 1.00 12.71
ATOM	563 CA ASP 231	-4.951 3.496 14.603 1.00 12.71
ATOM	564 CB ASP 231	-4.529 4.596 13.624 1.00 27.08
ATOM	565 CG ASP 231	-5.053 5.967 14.020 1.00 27.08
ATOM	566 OD1 ASP 231	-6.144 6.047 14.624 1.00 27.08
		0.21. 0.01. 11.027 1.00 27.00

ATOM	567 OD2 ASP 231	-4.370 6.969 13.723 1.00 27.08
ATOM	568 C ASP 231	-4.570 2.132 14.049 1.00 12.71
ATOM	569 O ASP 231	-5.413 1.436 13.483 1.00 27.08
ATOM	570 N PHE 232	-3.305 1.755 14.215 1.00 14.33
ATOM	571 CA PHE 232	-2.823 0.461 13.748 1.00 14.33
ATOM	572 CB PHE 232	-1.351 0.257 14.134 1.00 16.35
ATOM	573 CG PHE 232	-0.911 -1.184 14.097 1.00 16.35
ATOM	574 CD1 PHE 232	-0.789 -1.862 12.887 1.00 16.35
ATOM	575 CD2 PHE 232	-0.661 -1.879 15.280 1.00 16.35
ATOM	576 CE1 PHE 232	-0.430 -3.208 12.851 1.00 16.35
ATOM	577 CE2 PHE 232	-0.302 -3.224 15.255 1.00 16.35
ATOM	578 CZ PHE 232	-0.187 -3.890 14.038 1.00 16.35
ATOM	579 C PHE 232	-3.670 -0.642 14.368 1.00 14.33
ATOM	580 O PHE 232	-4.226 -1.482 13.661 1.00 16.35
ATOM	581 N ALA 233	-3.769 -0.619 15.695 1.00 15.30
ATOM	.582 CA ALA 233	-4.537 -1.607 16.444 1.00 15.30
ATOM	583 CB ALA 233	-4.413 -1.335 17.938 1.00 12.88
ATOM	584 C ALA 233	-6.005 -1.609 16.030 1.00 15.30
ATOM	585 O ALA 233	-6.627 -2.663 15.902 1.00 12.88
ATOM	586 N LYS 234	-6.542 -0.419 15.795 1.00 25.69
ATOM	587 CA LYS 234	-7.933 -0.256 15.401 1.00 25.69
ATOM	588 CB LYS 234	-8.270 1.234 15.318 1.00 45.91
ATOM	589 CG LYS 234	-9.574 1.595 15.979 1.00 45.91
ATOM	590 CD LYS 234	-9.535 1.268 17.463 1.00 45.91
ATOM	591 CE LYS 234	-10.938 1.047 18.006 1.00 45.91
ATOM	592 NZ LYS 234	-11.605 -0.106 17.327 1.00 45.91
ATOM	593 C LYS 234	-8.240 -0.931 14.067 1.00 25.69
ATOM	594 O LYS 234	-9.368 -1.368 13.827 1.00 45.91
ATOM	595 N LYS 235	-7.234 -1.019 13.204 1.00 17.44
ATOM	596 CA LYS 235	-7.406 -1.627 11.892 1.00 17.44
ATOM	597 CB LYS 235	-6.459 -0.975 10.884 1.00 26.26
ATOM	598 CG LYS 235	-6.757 0.499 10.669 1.00 26.26
ATOM ATOM	599 CD LYS 235	-5.785 1.141 9.706 1.00 26.26
ATOM	600 CE LYS 235 601 NZ LYS 235	-6.154 2.593 9.460 1.00 26.26 5.221 2.220 8.484 1.00 26.26
ATOM	601 NZ LYS 235 602 C LYS 235	-5.231 3.230 8.484 1.00 26.26 -7.258 -3.146 11.875 1.00 17.44
ATOM	603 O LYS 235	-7.256 -3.146 11.873 1.00 17.44 -7.365 -3.773 10.817 1.00 26.26
ATOM	604 N LEU 236	-7.015 -3.738 13.040 1.00 21.99
ATOM	605 CA LEU 236	-6.880 -5.187 13.144 1.00 21.99
ATOM	606 CB LEU 236	-5.792 -5.564 14.154 1.00 25.38
ATOM	607 CG LEU 236	-4.362 -5.127 13.818 1.00 25.38
ATOM	608 CD1 LEU 236	-3.415 -5.555 14.929 1.00 25.38
ATOM	609 CD2 LEU 236	-3.931 -5.725 12.491 1.00 25.38
ATOM	610 C LEU 236	-8.219 -5.796 13.556 1.00 21.99
ATOM	611 O LEU 236	-8.821 -5.386 14.553 1.00 25.38
ATOM	612 N PRO 237	-8.682 -6.819 12.817 1.00 34.89
ATOM	613 CD PRO 237	-7.936 -7.474 11.730 1.00 42.99
	AND HO!	11./50 1.00 42.77

ATOM 614 CA PRO 237 -9.953 -7.513 13.071 1.00 34.89 **ATOM** 615 CB PRO 237 -9.911 -8.687 12.084 1.00 42.99 **ATOM** 616 CG PRO 237 -8.433 -8.887 11.816 1.00 42.99 **ATOM** 617 C PRO 237 -10.184 -7.986 14.513 1.00 34.89 **ATOM** 618 O PRO 237 -11.142 -7.563 15.159 1.00 42.99 **ATOM** 619 N. MET 238 -9.301 -8.843 15.021 1.00 40.45 **ATOM** 620 CA MET 238 -9.433 -9.364 16.382 1.00 40.45 **ATOM** 621 CB MET 238 -8.360 -10.423 16.671 1.00 59.70 **ATOM** 622 CG MET 238 -8.689 -11.839 16.195 1.00 59.70 **ATOM** 623 SD MET 238 -8.013 -12.275 14.573 1.00 59.70 **ATOM** 624 CE MET 238 -6.482 -13.074 15.032 1.00 59.70 **ATOM** 625 C **MET** 238 -9.395 -8.305 17.486 1.00 40.45 **ATOM** 626 O **MET** 238 -9.801 -8.574 18.617 1.00 59.70 **ATOM** 627 N PHE 239 -8.928 -7.103 17.160 1.00 33.70 **ATOM** 628 CA PHE 239 -8.829 -6.037 18.152 1.00 33.70 **ATOM** 629 CB PHE 239 -7.651 -5.113 17.829 1.00 22.27 **ATOM** 630 CG PHE 239 -7.386 -4.079 18.885 1.00 22.27 **ATOM** 631 CD1 PHE 239 -6.602 -4.385 19.990 1.00 22.27 **ATOM** 632 CD2 PHE 239 -7.926 -2.802 18.778 1.00 22.27 **ATOM** 633 CE1 PHE 239 -6.358 -3.436 20.974 1.00 22.27 **ATOM** 634 CE2 PHE 239 -7.688 -1.846 19.757 1.00 22.27 635 CZ PHE **ATOM** 239 -6.901 -2.163 20.857 1.00 22.27 **ATOM** 636 C PHE 239 -10.103 -5.213 18.329 1.00 33.70 **ATOM** 637 O PHE 239 -10.594 -5.059 19.446 1.00 22.27 **ATOM** 638 N SER 240 -10.629 -4.679 17.232 1.00 23.42 **ATOM** 639 CA SER 240 -11.837 -3.857 17.278 1.00 23.42 **ATOM** 640 CB SER 240 -12.175 -3.352 15.884 1.00 26.21 **ATOM** 641 C SER 240 -13.046 -4.562 17.899 1.00 23.42 **ATOM** 642 O SER 240 -13.976 -3.909 18.369 1.00 26.21 643 N GLU **ATOM** 241 -13.028 -5.891 17.893 1.00 26.54 **ATOM** 644 CA GLU 241 -14.116 -6.695 18.450 1.00 26.54 **ATOM** 645 CB GLU 241 -14.007 -8.139 17.957 1.00 67.32 **ATOM** 646 CG GLU 241 -14.241 -8.322 16.467 1.00 67.32 **ATOM** 647 CD GLU 241 -13.979 -9.748 16.001 1.00 67.32 **ATOM** 648 OE1 GLU 241 -14.161 -10.691 16.803 1.00 67.32 **ATOM** 649 OE2 GLU 241 -13.584 -9.924 14.828 1.00 67.32 **ATOM** 650 C GLU 241 -14.137 -6.706 19.975 1.00 26.54 **ATOM** 651 O GLU 241 -15.182 -6.924 20.589 1.00 67.32 **ATOM** 652 N LEU 242 -12.972 -6.506 20.579 1.00 26.16 653 CA LEU 242 **ATOM** -12.835 -6.514 22.030 1.00 26.16 **ATOM** 654 CB LEU 242 -11.352 -6.473 22.412 1.00 19.79 **ATOM** 655 CG LEU 242 -10.461 -7.627 21.956 1.00 19.79 **ATOM** 242 656 CD1 LEU -9.014 -7.309 22.264 1.00 19.79 **ATOM** 657 CD2 LEU 242 -10.888 -8.912 22.640 1.00 19.79 **ATOM** 658 C LEU 242 -13.547 -5.351 22.711 1.00 26.16 **ATOM** 659 O LEU 242 -13.738 -4.290 22.115 1.00 19.79 **ATOM** 660 N PRO 243 -13.980 -5.547 23.968 1.00 17.98

ATOM	661 CD PRO 243	-13.996 -6.785 24.764 1.00 19.17
ATOM	662 CA PRO 243	-14.657 -4.454 24.671 1.00 17.98
ATOM	663 CB PRO 243	-15.095 -5.105 25.988 1.00 19.17
ATOM	664 CG PRO 243	-14.155 -6.263 26.161 1.00 19.17
ATOM	665 C PRO 243	-13.652 -3.323 24.898 1.00 17.98
ATOM	666 O PRO 243	-12.458 -3.572 25.081 1.00 19.17
ATOM	667 N CYS 244	-14.142 -2.088 24.880 1.00 20.08
ATOM	668 CA CYS 244	-13.310 -0.900 25.059 1.00 20.08
ATOM	669 CB CYS 244	-14.194 0.329 25.278 1.00 61.80
ATOM	670 SG CYS 244	-13.674 1.784 24.340 1.00 61.80
ATOM	671 C CYS 244	-12.286 -1.017 26.189 1.00 20.08
ATOM	672 O CYS 244	-11.141 -0.590 26.040 1.00 61.80
ATOM	673 N GLU 245	-12.691 -1.630 27.299 1.00 21.05
ATOM	674 CA GLU 245	-11.814 -1.811 28.454 1.00 21.05
ATOM	675 CB GLU 245	-12.541 -2.560 29.578 1.00 40.41
ATOM	676 CG GLU 245	-13.510 -1.705 30.393 1.00 40.41
ATOM	677 CD GLU 245	-14.953 -1.773 29.910 1.00 40.41
ATOM	678 OE1 GLU 245	-15.854 -1.761 30.775 1.00 40.41
ATOM	679 OE2 GLU 245	-15.197 -1.824 28.683 1.00 40.41
ATOM	680 C GLU 245	-10.541 -2.558 28.084 1.00 21.05
ATOM	681 O GLU 245	-9.439 -2.138 28.440 1.00 40.41
ATOM	682 N ASP 246	-10.698 -3.654 27.351 1.00 17.22
ATOM	683 CA ASP 246	-9.564 -4.463 26.924 1.00 17.22
ATOM	684 CB ASP 246	-10.044 -5.774 26.303 1.00 30.41
ATOM	685 CG ASP 246	-10.634 -6.727 27.327 1.00 30.41
ATOM	686 OD1 ASP 246	-10.755 -6.349 28.512 1.00 30.41
ATOM	687 OD2 ASP 246	-10.975 -7.864 26.946 1.00 30.41
ATOM	688 C ASP 246	-8.693 -3.705 25.936 1.00 17.22
ATOM	689 O ASP 246	-7.467 -3.713 26.050 1.00 30.41
ATOM	690 N GLN 247	-9.332 -3.045 24.973 1.00 17.12
ATOM	691 CA GLN 247	-8.615 -2.272 23.966 1.00 17.12
ATOM	692 CB GLN 247	-9.594 -1.494 23.088 1.00 16.72
ATOM	693 CG GLN 247	
ATOM	694 CD GLN 247	-11.352 -1.553 21.290 1.00 16.72
ATOM	695 OE1 GLN 247	-10.925 -0.515 20.790 1.00 16.72
ATOM	696 NE2 GLN 247	-12.560 -2.018 21.033 1.00 16.72
ATOM		-7.650 -1.303 24.637 1.00 17.12
ATOM	698 O GLN 247	-6.476 -1.228 24.273 1.00 16.72
ATOM	699 N ILE 248	-8.152 -0.591 25.640 1.00 19.19
ATOM	700 CA ILE 248	-7.358 0.377 26.387 1.00 19.19
ATOM	701 CB ILE 248	-8.238 1.137 27.410 1.00 24.32
ATOM	702 CG2 ILE 248	-7.385 2.055 28.282 1.00 24.32
ATOM	703 CG1 ILE 248	-9.312
ATOM	704 CD1 ILE 248	-10.327 2.618 27.573 1.00 24.32
ATOM	705 C ILE 248	-6.180 -0.297 27.093 1.00 19.19
ATOM	706 O ILE 248	-5.035 0.131 26.943 1.00 24.32
ATOM	707 N ILE 249	-6.457 -1.367 27.830 1.00 12.09

ATOM	708 CA ILE 249	-5.409 -2.090 28.547 1.00 12.09
ATOM	709 CB ILE 249	-5.996 -3.295 29.322 1.00 30.01
ATOM	710 CG2 ILE 249	-4.884 -4.168 29.885 1.00 30.01
ATOM	711 CG1 ILE 249	-6.899 -2.794 30.451 1.00 30.01
ATOM	712 CD1 ILE 249	-7.598 -3.893 31.215 1.00 30.01
ATOM	713 C ILE 249	-4.299 -2.561 27.602 1.00 12.09
ATOM	714 O ILE 249	-3.115 -2.339 27.866 1.00 30.01
ATOM	715 N LEU 250	-4.691 -3.168 26.486 1.00 20.87
ATOM	716 CA LEU 250	-3.740 -3.669 25.498 1.00 20.87
ATOM	717 CB LEU 250	-4.474 -4.410 24.376 1.00 15.15
ATOM	718 CG LEU 250	-5.252 -5.669 24.761 1.00 15.15
ATOM	719 CD1 LEU 250	-5.907 -6.256 23.533 1.00 15.15
ATOM	720 CD2 LEU 250	-4.325 -6.686 25.400 1.00 15.15
ATOM	721 C LEU 250	-2.900 -2.548 24.902 1.00 20.87
ATOM	722 O LEU 250	-1.680 -2.667 24.792 1.00 15.15
ATOM	723 N LEU 251	-3.559 -1.455 24.532 1.00 9.31
ATOM	724 CA LEU 251	-2.887 -0.301 23.945 1.00 9.31
ATOM	725 CB LEU 251	-3.920 0.760 23.553 1.00 19.90
ATOM	726 CG LEU 251	-4.075 1.127 22.073 1.00 19.90
ATOM	727 CD1 LEU 251	-3.281 0.190 21.180 1.00 19.90
ATOM	728 CD2 LEU 251	-5.550 1.113 21.699 1.00 19.90
ATOM	729 C LEU 251	-1.851 0.307 24.887 1.00 9.31
ATOM	730 O LEU 251	-0.699 0.521 24.507 1.00 19.90
ATOM	731 N LYS 252	-2.253 0.545 26.127 1.00 18.83
ATOM	732 CA LYS 252	-1.362 1.132 27.114 1.00 18.83
ATOM	733 CB LYS 252	-2.138 1.455 28.395 1.00 42.69
ATOM	734 CG LYS 252	-3.395 2.274 28.130 1.00 42.69
ATOM	735 CD LYS 252	-3.588 3.412 29.115 1.00 42.69
ATOM	736 CE LYS 252	-3.998 2.934 30.493 1.00 42.69
ATOM	737 NZ LYS 252	-4.300 4.109 31.361 1.00 42.69
ATOM	738 C LYS 252	-0.171 0.222 27.408 1.00 18.83
ATOM	739 O LYS 252	0.942 0.700 27.646 1.00 42.69
ATOM	740 N GLY 253	-0.392 -1.086 27.328 1.00 16.16
ATOM	741 CA GLY 253	0.676 -2.031 27.595 1.00 16.16
ATOM	742 C GLY 253	1.688 -2.232 26.479 1.00 16.16
ATOM .	743 O GLY 253	2.836 -2.587 26.747 1.00 34.57
ATOM	744 N CYS 254	1.286 -1.999 25.233 1.00 21.81
ATOM	745 CA CYS 254	2.194 -2.203 24.108 1.00 21.81
ATOM	746 CB CYS 254	1.563 -3.151 23.093 1.00 23.60
ATOM	747 SG CYS 254	0.211 -2.387 22.179 1.00 23.60
ATOM	748 C CYS 254	2.616 -0.935 23.380 1.00 21.81
ATOM	749 O CYS 254	3.499 -0.983 22.521 1.00 23.60
ATOM	750 N CYS 255	2.004 0.193 23.724 1.00 14.98
ATOM	751 CA CYS 255	2.309 1.461 23.066 1.00 14.98
ATOM	752 CB CYS 255	1.611 2.616 23.781 1.00 24.32
ATOM	753 SG CYS 255	1.602 4.153 22.841 1.00 24.32
ATOM	754 C CYS 255	3.804 1.750 22.922 1.00 14.98

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ATOM	755 O CYS 255	4.305 1.895 21.805 1.00 24.32
ATOM	756 N MET 256	4.525 1.777 24.037 1.00 13.77
ATOM	757 CA MET 256	5.959 2.056 24.003 1.00 13.77
ATOM	758 CB MET 256	6.515 2.218 25.423 1.00 19.23
ATOM	759 CG MET 256	7.988 2.607 25.477 1.00 19.23
ATOM	760 SD MET 256	8.344 4.132 24.571 1.00 19.23
ATOM	761 CE MET 256	10.127 4.254 24.782 1.00 19.23
ATOM	762 C MET 256	6.734 0.978 23.246 1.00 13.77
ATOM	763 O MET 256	7.672 1.284 22.516 1.00 19.23
ATOM	764 N GLU 257	6.316 -0.275 23.400 1.00 12.57
ATOM	765 CA GLU 257	6.971 -1.397 22.730 1.00 12.57
ATOM	766 CB GLU 257	6.342 -2.716 23.182 1.00 31.54
ATOM	767 CG GLU 257	6.497 -2.982 24.677 1.00 31.54
ATOM	768 CD GLU 257	5.720 -4.196 25.167 1.00 31.54
ATOM	769 OE1 GLU 257	5.220 -4.983 24.334 1.00 31.54
ATOM	770 OE2 GLU 257	5.607 -4.361 26.400 1.00 31.54
ATOM	771 C GLU 257	6.889 -1.254 21.211 1.00 12.57
ATOM	772 O GLU 257	7.881 -1.452 20.505 1.00 31.54
ATOM	773 N ILE 258	5.712 -0.881 20.717 1.00 17.89
ATOM	774 CA ILE 258	5.508 -0.692 19.288 1.00 17.89
ATOM ATOM	775 CB ILE 258 776 CG2 ILE 258	4.001 -0.555 18.946 1.00 15.57
ATOM	776 CG2 ILE 258 777 CG1 ILE 258	3.813 -0.129 17.493 1.00 15.57
ATOM	777 CG1 ILE 258	3.288 -1.886 19.211 1.00 15.57 1.798 -1.872 18.922 1.00 15.57
ATOM	778 CDI ILE 258	1.798 -1.872 18.922 1.00 15.57 6.289 0.535 18.811 1.00 17.89
ATOM	780 O ILE 258	7.000 0.468 17.805 1.00 15.57
ATOM	781 N MET 259	6.196 1.636 19.556 1.00 11.23
ATOM	782 CA MET 259	6.907 2.861 19.201 1.00 11.23
ATOM	783 CB MET 259	6.568 3.995 20.175 1.00 22.19
ATOM	784 CG MET 259	5.112 4.439 20.117 1.00 22.19
ATOM	785 SD MET 259	4.828 6.033 20.915 1.00 22.19
ATOM	786 CE MET 259	5.038 5.606 22.621 1.00 22.19
ATOM	787 C MET 259	8.415 2.637 19.131 1.00 11.23
ATOM	788 O MET 259	9.060 3.008 18.145 1.00 22.19
ATOM	789 N SER 260	8.974 1.994 20.153 1.00 8.59
ATOM	790 CA SER 260	10.408 1.706 20.195 1.00 8.59
ATOM	791 CB SER 260	10.763 0.939 21.472 1.00 23.39
ATOM	792 OG SER 260	10.430 1.685 22.623 1.00 23.39
ATOM	793 C SER 260	10.793 0.864 18.977 1.00 8.59
ATOM	794 O SER 260	11.824 1.100 18.350 1.00 23.39
ATOM	795 N LEU 261	9.952 -0.111 18.644 1.00 13.26
ATOM	796 CA LEU 261	10.194 -0.992 17.507 1.00 13.26
ATOM	797 CB LEU 261	9.076 -2.035 17.401 1.00 14.32
ATOM	798 CG LEU 261	9.019 -2.894 16.134 1.00 14.32
ATOM ATOM	799 CD1 LEU 261	10.278 -3.733 15.999 1.00 14.32
ATOM	800 CD2 LEU 261	7.785 -3.772 16.174 1.00 14.32
VIOM	801 C LEU 261	10.276 -0.170 16.220 1.00 13.26

ATOM	802 O LEU 261	11.213 -0.313 15.432 1.00 14.32
ATOM	803 N ARG 262	9.330 0.744 16.043 1.00 10.57
ATOM	804 CA ARG 262	9.278 1.598 14.861 1.00 10.57
ATOM	805 CB ARG 262	8.018 2.454 14.917 1.00 16.08
ATOM	806 CG ARG 262	6.755 1.647 14.728 1.00 16.08
ATOM	807 CD ARG 262	5.540 2.525 14.614 1.00 16.08
ATOM	808 NE ARG 262	4.418 1.765 14.076 1.00 16.08
ATOM	809 CZ ARG 262	3.260 2.289 13.689 1.00 16.08
ATOM	810 NH1 ARG 262	3.050 3.596 13.780 1.00 16.08
ATOM	811 NH2 ARG 262	2.322 1.497 13.183 1.00 16.08
ATOM	812 C ARG 262	10.530 2.471 14.704 1.00 10.57
ATOM	813 O ARG 262	11.038 2.649 13.589 1.00 16.08
ATOM	814 N ALA 263	11.016 3.014 15.820 1.00 13.37
ATOM	815 CA ALA 263	12.221 3.842 15.831 1.00 13.37
ATOM	816 CB ALA 263	12.363 4.516 17.172 1.00 17.12
ATOM	817 C ALA 263	13.443 2.964 15.561 1.00 13.37
ATOM	818 O ALA 263	14.313 3.316 14.762 1.00 17.12
ATOM	819 N ALA 264	13.474 1.802 16.207 1.00 16.55
ATOM	820 CA ALA 264	14.574 0.855 16.072 1.00 16.55
ATOM	821 CB ALA 264	14.375 -0.327 17.019 1.00 24.62
ATOM	822 C ALA 264	14.770 0.364 14.642 1.00 16.55
ATOM	823 O ALA 264	15.904 0.244 14.169 1.00 24.62
ATOM	824 N VAL 265	13.670 0.073 13.955 1.00 22.25
ATOM	825 CA VAL 265	13.754 -0.401 12.583 1.00 22.25
ATOM	826 CB VAL 265	12.428 -1.038 12.086 1.00 25.31
ATOM	827 CG1 VAL 265	12.079 -2.239 12.936 1.00 25.31
ATOM	828 CG2 VAL 265	11.302 -0.030 12.091 1.00 25.31
ATOM	829 C VAL 265	14.208 0.707 11.639 1.00 22.25
ATOM	830 O VAL 265	14.615 0.434 10.513 1.00 25.31
ATOM	831 N ARG 266	14.124 1.955 12.092 1.00 26.45
ATOM	832 CA ARG 266	14.567 3.086 11.283 1.00 26.45
ATOM	833 CB ARG 266	13.596 4.261 11.399 1.00 38.04
ATOM	834 CG ARG 266	12.232 4.019 10.807 1.00 38.04
ATOM	835 CD ARG 266	11.503 5.339 10.651 1.00 38.04
ATOM	836 NE ARG 266	10.074 5.216 10.925 1.00 38.04
ATOM	837 CZ ARG 266	9.504 5.551 12.079 1.00 38.04
ATOM	838 NH1 ARG 266	10.237 6.038 13.075 1.00 38.04
ATOM	839 NH2 ARG 266	8.196 5.411 12.240 1.00 38.04
ATOM	840 C ARG 266	15.957 3.531 11.729 1.00 26.45
ATOM	841 O ARG 266	16.296 4.717 11.660 1.00 38.04
ATOM	842 N TYR 267	16.733 2.590 12.251 1.00 24.87
ATOM	843 CA TYR 267	18.083 2.888 12.700 1.00 24.87
ATOM	844 CB TYR 267	18.592 1.788 13.639 1.00 25.84
ATOM	845 CG TYR 267	20.073 1.865 13.931 1.00 25.84
ATOM	846 CD1 TYR 267	20.579 2.789 14.844 1.00 25.84
ATOM	847 CE1 TYR 267	21.940 2.865 15.103 1.00 25.84
ATOM	848 CD2 TYR 267	20.971 1.017 13.284 1.00 25.84
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ATOM 849 CE2 TYR 267 22.331 1.085 13.536 1.00 25.84 **ATOM** 850 CZ TYR 267 22.810 2.011 14.444 1.00 25.84 **ATOM** 851 OH TYR 267 24.162 2.078 14.683 1.00 25.84 **ATOM** 852 C TYR 267 18.999 3.009 11.488 1.00 24.87 **ATOM** 853 O TYR 267 19.019 2.130 10.625 1.00 25.84 **ATOM** 854 N° ASP 268 19.751 4.102 11.423 1.00 28.13 **ATOM** 855 CA ASP 268 20.666 4.320 10.313 1.00 28.13 **ATOM** 856 CB ASP 268 20.524 5.744 9.773 1.00 51.63 **ATOM** 857 CG ASP 268 21.339 5.973 8.517 1.00 51.63 **ATOM** 858 OD1 ASP 268 21.060 5.305 7.498 1.00 51.63 **ATOM** 859 OD2 ASP 268 22.262 6.814 8.547 1.00 51.63 **ATOM** 860 C **ASP** 268 22.105 4.068 10.749 1.00 28.13 **ATOM** 861 O **ASP** 268 22.683 4.854 11.500 1.00 51.63 **ATOM PRO** 862 N 269 22.707 2.964 10.276 1.00 37.07 **ATOM** 863 CD PRO 269 22.103 1.938 9.410 1.00 39.18 **ATOM** 864 CA PRO 269 24.086 2.612 10.623 1.00 37.07 **ATOM** 865 CB PRO 269 24.319 1.324 9.832 1.00 39.18 **ATOM** 866 CG PRO 269 22.950 0.735 9.706 1.00 39.18 **ATOM** 867 C **PRO** 269 25.079 3.698 10.216 1.00 37.07 **PRO ATOM** 868 O 269 26.003 4.006 10.964 1.00 39.18 **ATOM** 869 N ALA 270 24.855 4.295 9.047 1.00 46.88 **ATOM** 870 CA ALA 270 25.730 5.340 8.519 1.00 46.88 **ATOM** 871 CB ALA 270 25.177 5.873 7.198 1.00 41.71 **ATOM** 872 C ALA 270 25.974 6.493 9.492 1.00 46.88 **ATOM** 873 O ALA 270 27.121 6.844 9.763 1.00 41.71 **ATOM** 874 N SER 7.081 10.009 1.00 34.54 271 24.899 **ATOM** 875 CA SER 271 25.013 8.198 10.941 1.00 34.54 23.959 9.259 10.618 1.00 42.29 **ATOM** 876 CB SER 271 **ATOM** 877 OG SER 271 22.686 8.668 10.422 1.00 42.29 **ATOM** 878 C SER 271 24.910 7.793 12.408 1.00 34.54 **ATOM** 879 O SER 271 25.169 8.607 13.297 1.00 42.29 **ATOM** 880 N **ASP** 272 24.546 6.535 12.653 1.00 41.05 **ATOM** 881 CA ASP 272 24.388 6.005 14.007 1.00 41.05 **ATOM** 882 CB ASP 272 25.720 6.078 14.772 1.00 47.32 **ATOM** 883 CG ASP 272 25.653 5.428 16.147 1.00 47.32 **ATOM** 884 OD1 ASP 272 24.981 4.384 16.299 1.00 47.32 **ATOM** 885 OD2 ASP 272 26.284 5.967 17.081 1.00 47.32 **ASP ATOM** 886 C 272 23.279 6.777 14.730 1.00 41.05 **ASP ATOM** 887 O 272 23.444 7.233 15.866 1.00 47.32 273 **ATOM** 888 N THR 22.139 6.905 14.058 1.00 27.60 **ATOM** 889 CA THR 273 20.996 7.618 14.608 1.00 27.60 **ATOM** 890 CB THR 273 20.808 8.991 13.911 1.00 30.96 **ATOM** 891 OG1 THR 273 20.723 8.808 12.491 1.00 30.96 **ATOM** 892 CG2 THR 273 21.967 9.924 14.228 1.00 30.96 **ATOM** 893 C THR 273 19.701 6.829 14.442 1.00 27.60 **ATOM** 894 O THR 273 19.633 5.883 13.650 1.00 30.96 **ATOM** 895 N LEU 274 18.696 7.192 15.232 1.00 20.89

ATOM 896 CA LEU 274 17.374 6.574 15.161 1.00 20.89 **ATOM** 897 CB LEU 274 16.862 6.193 16.555 1.00 22.48 **ATOM** 898 CG LEU 274 17.480 5.009 17.301 1.00 22.48 **ATOM** 899 CD1 LEU 274 4.866 18.650 1.00 22.48 16.798 **ATOM** 900 CD2 LEU 274 17.317 3.736 16.497 1.00 22.48 **ATOM** 901 C. LEU 274 16.470 7.654 14.586 1.00 20.89 **ATOM** 902 O LEU 274 8.842 14.744 1.00 22.48 16.753 903 N **ATOM** THR 275 15.393 7.258 13.922 1.00 27.89 **ATOM** 904 CA THR 275 14.478 8.235 13.354 1.00 27.89 **ATOM** 905 CB THR 275 14.325 8.045 11.832 1.00 37.64 **ATOM** 906 OG1 THR 275 15.622 7.983 11.228 1.00 37.64 **ATOM** 907 CG2 THR 275 13.570 9.215 11.222 1.00 37.64 **ATOM** 908 C THR 275 13.120 8.135 14.032 1.00 27.89 **ATOM** 909 O THR 275 12.493 7.081 14.019 1.00 37.64 **ATOM** 910 N LEU 276 12.700 9.226 14.667 1.00 28.07 **ATOM** 911 CA LEU 276 11.418 9.275 15.358 1.00 28.07 **ATOM** 912 CB LEU 276 11.497 10.214 16.572 1.00 24.81 **ATOM** 913 CG LEU 276 12.639 10.005 17.577 1.00 24.81 **ATOM** 914 CD1 LEU 276 12.450 10.929 18.769 1.00 24.81 915 CD2 LEU **ATOM** 276 12.692 8.558 18.038 1.00 24.81 **ATOM** 916 C LEU 276 10.339 9.761 14.395 1.00 28.07 **ATOM** 917 O LEU 276 10.533 10.760 13.691 1.00 24.81 **ATOM** 918 N SER 277 9.232 9.027 14.331 1.00 29.24 **ATOM** 919 CA SER 277 8.106 9.357 13.458 1.00 29.24 **ATOM** 920 CB SER 277 7.369 10.594 13.985 1.00 30.56 **ATOM** 921 OG SER 277 6.845 10.358 15.283 1.00 30.56 **ATOM** 922 C SER 277 8.533 9.569 12.005 1.00 29.24 **ATOM** 923 O SER 277 7.902 10.326 11.263 1.00 30.56 **ATOM** 924 N GLY 278 9.619 8.908 11.618 1.00 34.41 **ATOM** 925 CA GLY 278 10.135 9.024 10.263 1.00 34.41 **ATOM** 926 C **GLY** 278 10.472 10.442 9.830 1.00 34.41 ATOM 927 O **GLY** 278 10.516 10.725 8.631 1.00 44.04 **ATOM** 928 N **GLU** 279 10.733 11.326 10.791 1.00 37.82 **ATOM** 929 CA GLU 279 11.056 12.717 10.479 1.00 37.82 **ATOM** 930 CB GLU 279 9.808 13.600 10.612 1.00 70.24 **ATOM** 931 CG GLU 279 9.202 13.631 12.014 1.00 70.24 **ATOM** 932 CD GLU 279 8.028 14.593 12.141 1.00 70.24 279 **ATOM** 933 OE1 GLU 8.028 15.406 13.093 1.00 70.24 **ATOM** 279 934 OE2 GLU 7.103 14.535 11.301 1.00 70.24 **ATOM** 935 C GLU 279 12.192 13.321 11.300 1.00 37.82 936 O 279 ATOM GLU 12.857 14.248 10.841 1.00 70.24 **ATOM** 937 N MET 280 12.424 12.811 12.505 1.00 33.77 938 CA MET **ATOM** 280 13.482 13.360 13.344 1.00 33.77 **ATOM 939 CB MET** 280 12.903 13.848 14.674 1.00 33.89 **ATOM** 940 CG MET 280 13.898 14.595 15.545 1.00 33.89 **ATOM** 941 SD MET 280 13.350 14.740 17.256 1.00 33.89 **ATOM 942 CE MET** 280 12.100 16.017 17.121 1.00 33.89

ATOM	943 C MET 280	14.620 12.383 13.613 1.00 33.77
ATOM	944 O MET 280	14.432 11.366 14.282 1.00 33.89
ATOM	945 N ALA 281	15.797 12.690 13.080 1.00 30.24
ATOM	946 CA ALA 281	16.972 11.852 13.287 1.00 30.24
ATOM	947 CB ALA 281	17.937 11.998 12.120 1.00 25.10
ATOM	948 C ALA 281	17.631 12.309 14.587 1.00 30.24
ATOM	949 O ALA 281	18.008 13.477 14.718 1.00 25.10
ATOM	950 N VAL 282	17.743 11.401 15.551 1.00 32.12
ATOM	951 CA VAL 282	18.339 11.726 16.844 1.00 32.12
ATOM	952 CB VAL 282	17.303 11.606 17.991 1.00 37.75
ATOM	953 CG1 VAL 282	16.184 12.615 17.799 1.00 37.75
ATOM	954 CG2 VAL 282	16.739 10.193 18.055 1.00 37.75
ATOM	955 C VAL 282	19.543 10.852 17.181 1.00 32.12
ATOM	956 O VAL 282	19.614 9.690 16.778 1.00 37.75
ATOM	957 N LYS 283	20.491 11.428 17.913 1.00 26.82
ATOM	958 CA LYS 283	21.700 10.722 18.328 1.00 26.82
ATOM	959 CB LYS 283	22.894 11.679 18.342 1.00 57.25
ATOM	960 CG LYS 283	23.258 12.245 16.979 1.00 57.25
ATOM	961 CD LYS 283	24.282 13.361 17.105 1.00 57.25
ATOM	962 CE LYS 283	24.752 13.836 15.741 1.00 57.25
ATOM	963 NZ LYS 283	25.518 12.772 15.033 1.00 57.25
ATOM	964 C LYS 283	21.509 10.120 19.717 1.00 26.82
ATOM	965 O LYS 283	20.648 10.566 20.477 1.00 57.25
ATOM	966 N ARG 284	22.351 9.146 20.058 1.00 26.41
ATOM	967 CA ARG 284	22.297 8.457 21.351 1.00 26.41
ATOM	968 CB ARG 284	23.527 7.566 21.528 1.00 41.02
ATOM	969 CG ARG 284	23.715 6.539 20.440 1.00 41.02
ATOM	970 CD ARG 284	25.016 5.794 20.616 1.00 41.02
ATOM	971 NE ARG 284	25.145 4.730 19.630 1.00 41.02
ATOM	972 CZ ARG 284	24.759 3.475 19.831 1.00 41.02
ATOM	973 NH1 ARG 284	24.221 3.117 20.990 1.00 41.02
ATOM	974 NH2 ARG 284	24.886 2.584 18.859 1.00 41.02
ATOM	975 C ARG 284	22.200 9.399 22.543 1.00 26.41
ATOM	976 O ARG 284	21.296 9.278 23.370 1.00 41.02
ATOM	977 N GLU 285	23.152 10.321 22.634 1.00 33.23
ATOM	978 CA GLU 285	23.201 11.292 23.721 1.00 33.23
ATOM	979 CB GLU 285	24.366 12.258 23.492 1.00 69.82
ATOM	980 CG GLU 285	24.485 13.359 24.533 1.00 69.82
ATOM	981 CD GLU 285	25.079 14.636 23.964 1.00 69.82
ATOM	982 OE1 GLU 285	26.309 14.826 24.070 1.00 69.82
ATOM	983 OE2 GLU 285	24.309 15.453 23.409 1.00 69.82
ATOM	984 C GLU 285	21.898 12.082 23.823 1.00 33.23
ATOM	985 O GLU 285	21.336 12.239 24.907 1.00 69.82
ATOM	986 N GLN 286	21.414 12.551 22.677 1.00 28.07
ATOM	987 CA GLN 286	20.194 13.346 22.614 1.00 28.07
ATOM	988 CB GLN 286	19.948 13.824 21.181 1.00 41.05
ATOM	989 CG GLN 286	21.051 14.726 20.639 1.00 41.05
		•

ATOM 990 CD GLN 286 20.808 15.154 19.202 1.00 41.05 **ATOM** 991 OE1 GLN 286 20.783 14.322 18.293 1.00 41.05 **ATOM** 992 NE2 GLN 286 20.635 16.452 18.990 1.00 41.05 **ATOM** 993 C GLN 286 18.955 12.642 23.162 1.00 28.07 **ATOM** 994 O GLN 286 18.281 13.174 24.048 1.00 41.05 **ATOM** 995 N. LEU 287 18.663 11.447 22.658 1.00 30.11 **ATOM** 996 CA LEU 287 17.492 10.705 23.116 1.00 30.11 **ATOM** 997 CB LEU 287 17.232 9.489 22.219 1.00 21.70 **ATOM** 998 CG LEU 287 8.821 22.357 1.00 21.70 15.859 **ATOM** 999 CD1 LEU 287 14.748 9.818 22.061 1.00 21.70 **ATOM** 1000 CD2 LEU 287 15.763 7.628 21.421 1.00 21.70 **ATOM** 1001 C LEU 287 17.641 10.277 24.577 1.00 30.11 1002 O LEU 287 ATOM 16.655 10.212 25.320 1.00 21.70 **ATOM** 1003 N LYS 288 18.878 10.015 24.992 1.00 20.72 **ATOM** 1004 CA LYS 288 19.156 9.611 26.365 1.00 20.72 **ATOM** 1005 CB LYS 288 20.626 9.213 26.514 1.00 43.14 **ATOM** 1006 CG LYS 288 20.991 8.721 27.903 1.00 43.14 ATOM 1007 CD LYS 288 22.374 8.102 27.931 1.00 43.14 **ATOM** 1008 CE LYS 288 22.615 7.379 29.250 1.00 43.14 ATOM 1009 NZ LYS 288 23.866 6.568 29.224 1.00 43.14 **ATOM** 1010 C LYS 288 18.819 10.742 27.331 1.00 20.72 **ATOM** LYS 1011 O 288 18.027 10.566 28.261 1.00 43.14 **ATOM** 1012 N **ASN** 289 19.380 11.917 27.067 1.00 33.64 **ATOM** 1013 CA ASN 289 19.156 13.090 27.906 1.00 33.64 **ATOM** 1014 CB ASN 289 20.190 14.173 27.590 1.00 35.61 ATOM 1015 CG ASN 289 21.607 13.730 27.898 1.00 35.61 **ATOM** 289 1016 OD1 ASN 21.835 12.920 28.797 1.00 35.61 **ATOM** 1017 ND2 ASN 289 22.566 14.253 27.149 1.00 35.61 **ATOM** 1018 C **ASN** 289 17.747 13.654 27.757 1.00 33.64 **ATOM** 1019 O ASN 289 17.276 14.399 28.616 1.00 35.61 1020 N **ATOM GLY** 290 17.072 13.287 26.672 1.00 22.05 **ATOM** 1021 CA GLY 290 15.722 13.767 26.435 1.00 22.05 **ATOM** 1022 C GLY 290 14.688 13.247 27.416 1.00 22.05 **ATOM** 1023 O GLY 290 13.550 13.710 27.420 1.00 29.95 **ATOM** 1024 N GLY 291 15.072 12.276 28.239 1.00 24.91 **ATOM** 1025 CA GLY 291 14.142 11.732 29.211 1.00 24.91 **ATOM** 1026 C GLY 291 14.093 10.217 29.248 1.00 24.91 **ATOM** 1027 O **GLY** 291 13.536 9.640 30.179 1.00 29.39 1028 N LEU **ATOM** 292 14.676 9.567 28.246 1.00 30.21 **ATOM** 1029 CA LEU 292 14.675 8.110 28.189 1.00 30.21 **ATOM** 1030 CB LEU 292 14.732 7.626 26.734 1.00 21.45 1031 CG LEU **ATOM** 292 13.439 7.795 25.928 1.00 21.45 **ATOM** 1032 CD1 LEU 292 7.225 24.542 1.00 21.45 13.612 **ATOM** 292 12.296 7.087 26.630 1.00 21.45 1033 CD2 LEU **ATOM** 1034 C LEU 292 15.785 7.461 29.013 1.00 30.21 **ATOM** 1035 O LEU 292 15.645 6.324 29.473 1.00 21.45 **ATOM** 1036 N GLY 293 16.885 8.180 29.205 1.00 16.29

ATOM 1037 CA GLY 293 17.992 7.638 29.970 1.00 16.29 1038 C **ATOM GLY** 18.534 6.374 29.332 1.00 16.29 293 **ATOM** 1039 O GLY 293 6.334 28.122 1.00 25.88 18.763 **ATOM** 1040 N VAL 294 18.689 5.322 30.130 1.00 33.05 **ATOM** 1041 CA VAL 294 19.211 4.050 29.635 1.00 33.05 **ATOM** 1042 CB VAL 294 19.530 3.069 30.788 1.00 30.11 ATOM 1043 CG1 VAL 294 20.718 3.577 31.582 1.00 30.11 **ATOM** 1044 CG2 VAL 294 18.315 2.887 31.697 1.00 30.11 ATOM 1045 C VAL 294 18.302 3.361 28.617 1.00 33.05 ATOM 1046 O VAL 294 18.768 2.545 27.817 1.00 30.11 **ATOM** 1047 N VAL 295 17.014 3.699 28.635 1.00 18.14 ATOM 1048 CA VAL 295 16.056 3.118 27.698 1.00 18.14 **ATOM** 1049 CB VAL 295 14.638 3.698 27.902 1.00 28.34 1050 CG1 VAL 295 ATOM 13.668 3.099 26.893 1.00 28.34 **ATOM** 1051 CG2 VAL 295 14.159 3.431 29.317 1.00 28.34 **ATOM** 1052 C VAL 295 16.521 3.415 26.275 1.00 18.14 1053 O VAL 295 **ATOM** 16.395 2.577 25.383 1.00 28.34 1054 N SER 296 **ATOM** 17.091 4.601 26.085 1.00 20.84 1055 CA SER ATOM 296 17.596 5.028 24.785 1.00 20.84 ATOM 1056 CB SER 296 18.160 6.446 24.884 1.00 25.61 **ATOM** 1057 OG SER 296 18.615 6.911 23.627 1.00 25.61 **ATOM** 1058 C SER 296 18.687 4.074 24.307 1.00 20.84 **ATOM** 1059 O **SER** 296 18.723 3.691 23.133 1.00 25.61 ATOM 1060 N **ASP** 297 19.571 3.691 25.224 1.00 28.08 20.660 2.777 24.904 1.00 28.08 **ATOM** 1061 CA ASP 297 **ATOM** 1062 CB ASP 297 21.555 2.552 26.129 1.00 51.15 ATOM 1063 CG ASP 297 22.207 3.835 26.629 1.00 51.15 **ATOM** 1064 OD1 ASP 297 22.508 4.725 25.804 1.00 51.15 ATOM 1065 OD2 ASP 297 22.425 3.948 27.855 1.00 51.15 ATOM 1066 C **ASP** 297 20.079 1.450 24.434 1.00 28.08 **ATOM** 1067 O **ASP** 297 20.549 0.869 23.456 1.00 51.15 **ATOM** 1068 N ALA 298 19.024 1.006 25.111 1.00 26.12 **ATOM** 1069 CA ALA 298 18.357 -0.245 24.778 1.00 26.12 **ATOM** 1070 CB ALA 298 17.253 -0.530 25.787 1.00 18.80 ATOM 1071 C ALA 298 17.790 -0.223 23:356 1.00 26.12 298 **ATOM** 1072 O ALA 18.014 -1.154 22.575 1.00 18.80 1073 N ILE 299 **ATOM** 17.078 0.848 23.013 1.00 17.42 1074 CA ILE 299 **ATOM** 16.483 0.979 21.686 1.00 17.42 1075 CB ILE 299 **ATOM** 15.559 2.211 21.597 1.00 16.69 1076 CG2 ILE 299 **ATOM** 14.845 2.238 20.253 1.00 16.69 **ATOM** 1077 CG1 ILE 299 14.515 2.149 22.712 1.00 16.69 **ATOM** 1078 CD1 ILE 299 13.713 3.406 22.872 1.00 16.69 **ATOM** 1079 C ILE 299 17.563 1.042 20.609 1.00 17.42 1080 O ILE 299 **ATOM** 17.416 0.443 19.542 1.00 16.69 1081 N PHE 300 **ATOM** 18.652 1.752 20.889 1.00 14.46 **ATOM** 1082 CA PHE 300 19.751 1.851 19.935 1.00 14.46 **ATOM** 1083 CB PHE 300 20.804 2.854 20.409 1.00 24.01

ATOM	1 1084 CG PHE 300	20.656 4.221 19.801 1.00 24.01
ATOM		19.904 5.204 20.435 1.00 24.01
ATOM		21.271 4.526 18.591 1.00 24.01
ATOM		19.766 6.472 19.873 1.00 24.01
ATOM		21.140 5.791 18.020 1.00 24.01
ATOM		20.385 6.765 18.663 1.00 24.01
ATOM		20.383 0.480 19.726 1.00 14.46
ATOM		20.696 0.102 18.596 1.00 24.01
ATOM		20.547 -0.270 20.813 1.00 21.61
ATOM		21.123 -1.609 20.744 1.00 21.61
ATOM		21.289 -2.192 22.143 1.00 23.89
ATOM		20.211 -2.498 19.904 1.00 21.61
ATOM		20.681 -3.251 19.043 1.00 23.89
ATOM		18.906 -2.390 20.140 1.00 14.43
ATOM		17.922 -3.168 19.399 1.00 14.43
ATOM ATOM		16.512 -2.872 19.912 1.00 23.43
ATOM		15.350 -3.669 19.312 1.00 23.43
ATOM	,	15.459 -5.140 19.688 1.00 23.43 14.035 -3.094 19.804 1.00 23.43
ATOM	· · · · · · · · · · · · · · · · · · ·	14.035 -3.094 19.804 1.00 23.43 18.027 -2.812 17.917 1.00 14.43
ATOM		18.089 -3.697 17.066 1.00 23.43
ATOM	1105 N GLY 303	18.098 -1.515 17.625 1.00 15.17
ATOM	1106 CA GLY 303	18.208 -1.056 16.251 1.00 15.17
ATOM	1107 C GLY 303	19.411 -1.640 15.530 1.00 15.17
ATOM	1108 O GLY 303	19.290 -2.137 14.406 1.00 27.67
ATOM	1109 N LYS 304	20.570 -1.594 16.182 1.00 19.04
ATOM	1110 CA LYS 304	21.802 -2.127 15.605 1.00 19.04
ATOM	1111 CB LYS 304	22.979 -1.975 16.577 1.00 56.94
ATOM	1112 CG LYS 304	23.496 -0.556 16.741 1.00 56.94
ATOM	1113 CD LYS 304	24.811 -0.524 17.516 1.00 56.94
ATOM	1114 CE LYS 304	24.634 -0.965 18.968 1.00 56.94
ATOM	1115 NZ LYS 304	23.838 0.008 19.778 1.00 56.94
ATOM	1116 C LYS 304	21.653 -3.596 15.229 1.00 19.04
ATOM	1117 O LYS 304	21.974 -3.993 14.107 1.00 56.94
ATOM	1118 N SER 305	21.146 -4.394 16:164 1.00 24.46
ATOM	1119 CA SER 305	20.965 -5.822 15.932 1.00 24.46
ATOM	1120 CB SER 305	20.610 -6.533 17.240 1.00 37.46
ATOM	1121 OG SER 305	19.444 -5.984 17.827 1.00 37.46
ATOM	1122 C SER 305	19.926 -6.128 14.853 1.00 24.46
ATOM ATOM	1123 O SER 305	20.146 -6.996 14.006 1.00 37.46
ATOM	1124 N LEU 306 1125 CA LEU 306	18.819 -5.390 14.858 1.00 25.47
ATOM		17.753 -5.592 13.881 1.00 25.47
ATOM	1126 CB LEU 306 1127 CG LEU 306	16.525 -4.746 14.224 1.00 15.99 15.700 -5.190 15.432 1.00 15.99
ATOM	1127 CG LEU 306	14.504 -4.271 15.600 1.00 15.99
ATOM	1128 CD1 LEU 306	15.244 -6.624 15.247 1.00 15.99
ATOM	1130 C LEU 306	18.174 -5.330 12.439 1.00 25.47
1110111	IIJO C EEO JOO	10.174 -5.550 12.455 1.00 25.47

ATOM 1131 O LEU 306 17.596 -5.902 11.513 1.00 15.99 **ATOM** 1132 N SER 307 19.182 -4.482 12.247 1.00 24.28 **ATOM** 1133 CA SER 307 19.670 -4.160 10.907 1.00 24.28 **ATOM** 1134 CB SER 307 20.910 -3.263 10.989 1.00 40.92 ATOM 1135 OG SER 307 20.617 -2.028 11.622 1.00 40.92 **ATOM** 1136 C SER 307 19.995 -5.422 10.107 1.00 24.28 **ATOM** 1137 O SER 307 19.625 -5.535 8.936 1.00 40.92 ATOM 1138 N 308 ALA 20.644 -6.383 10.761 1.00 30.97 **ATOM** 1139 CA ALA 308 21.027 -7.640 10.124 1.00 30.97 **ATOM** 1140 CB ALA 308 22.004 -8.399 11.013 1.00 37.84 **ATOM** 1141 C ALA 308 19.830 -8.528 9.779 1.00 30.97 **ATOM** 1142 O ALA 308 19.897 -9.336 8.853 1.00 37.84 **ATOM** PHE 309 1143 N 18.737 -8.372 10.520 1.00 22.78 1144 CA PHE **ATOM** 309 17.533 -9.166 10.292 1.00 22.78 ATOM 1145 CB PHE 309 16.571 -9.037 11.477 1.00 30.14 **ATOM** 1146 CG PHE 309 17.032 -9.751 12.716 1.00 30.14 **ATOM** 1147 CD1 PHE 309 16.299 -10.809 13.236 1.00 30.14 **ATOM** 1148 CD2 PHE 309 18.204 -9.372 13.359 1.00 30.14 **ATOM** 1149 CE1 PHE 309 16.725 -11.481 14.378 1.00 30.14 **ATOM** 1150 CE2 PHE 309 18.640 -10.038 14.503 1.00 30.14 ATOM 1151 CZ PHE 309 17.896 -11.094 15.013 1.00 30.14 **ATOM** 1152 C PHE 309 16.818 -8.813 8.990 1.00 22.78 **ATOM** 1153 O PHE 309 16.068 -9.631 8.451 1.00 30.14 ATOM 1154 N ASN 310 17.051 -7.598 8.496 1.00 35.30 **ATOM** 1155 CA ASN 310 16.441 -7.109 7.255 1.00 35.30 **ATOM** 1156 CB ASN 310 17.109 -7.760 6.037 1.00 28.28 **ATOM** 1157 C **ASN** 310 14.929 -7.339 7.229 1.00 35.30 **ATOM** 1158 O **ASN** 310 14.395 -7.970 6.312 1.00 28.28 **ATOM** 1159 N LEU 311 14.249 -6.831 8.251 1.00 27.52 ATOM 1160 CA LEU 311 12.803 -6.979 8.369 1.00 27.52 **ATOM** 1161 CB LEU 311 12.351 -6.630 9.788 1.00 22.62 ATOM 1162 CG LEU 311 12.950 -7.396 10.968 1.00 22.62 **ATOM** 1163 CD1 LEU 311 12.360 -6.864 12.268 1.00 22.62 **ATOM** 1164 CD2 LEU 311 12.672 -8.881 10.821 1.00 22.62 LEU **ATOM** 1165 C 311 12.060 -6.085 7.382 1.00 27.52 1166 O **ATOM** LEU 311 12.519 -4.986 7.067 1.00 22.62 **ATOM** 1167 N **ASP** 312 10.918 -6.563 6.892 1.00 16.74 312 **ATOM** 1168 CA ASP 10.095 -5.789 5.968 1.00 16.74 **ATOM** 1169 CB ASP 312 9.803 -6.578 4.673 1.00 16.35 **ATOM** 1170 CG ASP 312 8.924 -7.814 4.888 1.00 16.35 **ATOM** 1171 OD1 ASP 312 8.591 -8.168 6.037 1.00 16.35 **ATOM** 1172 OD2 ASP 312 8.559 -8.446 3.876 1.00 16.35 8.808 -5.354 6.678 1.00 16.74 **ATOM** 1173 C **ASP** 312 **ASP** 312 **ATOM** 1174 O 8.535 -5.798 7.797 1.00 16.35 **ATOM** 1175 N **ASP** 313 8.007 -4.520 6.019 1.00 5.43 **ATOM** 1176 CA ASP 313 6.758 -4.016 6.592 1.00 5.43 5.974 -3.201 5.559 1.00 31.80 **ATOM** 1177 CB ASP 313

ATOM 1178 CG ASP 313 6.670 -1.906 5.183 1.00 31.80 **ATOM** 1179 OD1 ASP 313 7.392 -1.340 6.033 1.00 31.80 1180 OD2 ASP 313 **ATOM** 6.493 -1.452 4.032 1.00 31.80 **ATOM** 1181 C ASP 313 5.849 -5.081 7.189 1.00 5.43 **ASP** ATOM 1182 O 313 5.216 -4.849 8.221 1.00 31.80 **ATOM** 1183 N THR 314 5.777 -6.238 6.543 1.00 12.98 **ATOM** 1184 CA THR 314 4.934 -7.327 7.022 1.00 12.98 **ATOM** 1185 CB THR 314 4.825 -8.441 5.968 1.00 18.90 ATOM 1186 OG1 THR 314 4.249 -7.904 4.769 1.00 18.90 ATOM 3.960 -9.578 1187 CG2 THR 314 6.477 1.00 18.90 ATOM 1188 C THR 314 5.426 -7.910 8.349 1.00 12.98 ATOM 1189 O THR 314 4.636 -8.124 9.268 1.00 18.90 **ATOM** 1190 N **GLU** 315 6.731 -8.135 8.457 1.00 9.13 **ATOM** 1191 CA GLU 315 7.316 -8.685 9.675 1.00 9.13 **ATOM** 1192 CB GLU 315 8.771 -9.078 9.427 1.00 11.49 **ATOM** 1193 CG GLU 315 8.870 -10.323 8.562 1.00 11.49 ATOM 1194 CD GLU 315 10.233 -10.544 7.945 1.00 11.49 ATOM 1195 OE1 GLU 315 10.964 -9.561 7.705 1.00 11.49 **ATOM** 1196 OE2 GLU 315 10.558 -11.715 7.669 1.00 11.49 **ATOM** 1197 C GLU 315 7.180 -7.720 10.847 1.00 9.13 ATOM 1198 O **GLU** 315 6.863 -8.131 11.967 1.00 11.49 **ATOM** 1199 N VAL 316 7.376 -6.433 10.575 1.00 9.46 **ATOM** 1200 CA VAL 316 7.240 -5.406 11.602 1.00 9.46 **ATOM** 1201 CB VAL 316 7.655 -4.015 11.063 1.00 7.95 **ATOM** 1202 CG1 VAL 316 7.434 -2.941 12.124 1.00 7.95 **ATOM** 1203 CG2 VAL 316 9.112 -4.037 10.625 1.00 7.95 1204 C **ATOM** VAL 316 5.777 -5.365 12.051 1.00 9.46 VAL ATOM 1205 O 316 5.484 -5.300 13.247 1.00 7.95 **ATOM** 1206 N ALA 317 4.866 -5.438 11.083 1.00 5.52 **ATOM** 1207 CA ALA 317 3.434 -5.417 11.355 1.00 5.52 1208 CB ALA **ATOM** 317 2.656 -5.415 10.054 1.00 10.98 **ATOM** 1209 C ALA 317 3.002 -6.595 12.225 1.00 5.52 **ATOM** 1210 O ALA 317 2.317 -6.412 13.230 1.00 10.98 **ATOM** 1211 N LEU 318 3.411 -7.799 11.838 1.00 8.62 **ATOM** 1212 CA LEU 318 3.067 -9.003 12.584 1.00 8.62 **ATOM** 1213 CB LEU 318 3.523 -10.249 11.825 1.00 10.49 **ATOM** 1214 CG LEU 318 2.770 -10.494 10.514 1.00 10.49 **ATOM** 1215 CD1 LEU 318 3.376 -11.664 9.769 1.00 10.49 **ATOM** 1216 CD2 LEU 318 1.297 -10.741 10.799 1.00 10.49 **ATOM** 1217 C LEU 318 3.674 -8.971 13.978 1.00 8.62 1218 O LEU 318 **ATOM** 3.047 -9.407 14.945 1.00 10.49 **ATOM** 1219 N LEU 319 4.885 -8.435 14.082 1.00 9.43 319 **ATOM** 1220 CA LEU 5.560 -8.325 15.366 1.00 9.43 **ATOM** 1221 CB LEU 319 6.975 -7.773 15.173 1.00 24.05 **ATOM** 1222 CG LEU 319 7.901 -7.680 16.389 1.00 24.05 **ATOM** 1223 CD1 LEU 319 7.889 -8.977 17.182 1.00 24.05 **ATOM** 1224 CD2 LEU 319 9.310 -7.356 15.922 1.00 24.05

ATO	M 1225 C LEU 319	4.731 -7.404 16.259 1.00 9.43
ATO	M 1226 O LEU 319	4.456 -7.731 17.416 1.00 24.05
ATO	M 1227 N GLN 320	4.287 -6.282 15.699 1.00 8.67
ATO	M 1228 CA GLN 320	3.467 -5.325 16.437 1.00 8.67
ATO	M 1229 CB GLN 320	3.151 -4.102 15.573 1.00 10.94
ATO:	M 1230 CG GLN 320	4.361 -3.256 15.218 1.00 10.94
ATO:	M 1231 CD GLN 320	4.025 -2.045 14.359 1.00 10.94
ATO	M 1232 OE1 GLN 320	4.889 -1.217 14.082 1.00 10.94
ATO	M 1233 NE2 GLN 320	2.773 -1.940 13.924 1.00 10.94
ATO	M 1234 C GLN 320	2.169 -5.984 16.895 1.00 8.67
ATO		1.708 -5.751 18.013 1.00 10.94
ATO		1.586 -6.806 16.028 1.00 9.21
ATO		0.349 -7.513 16.342 1.00 9.21
ATO		-0.136 -8.283 15.129 1.00 12.83
ATO		0.558 -8.460 17.523 1.00 9.21
ATO		-0.315 -8.591 18.382 1.00 12.83
ATO		1.718 -9.111 17.566 1.00 9.10
ATO		2.043 -10.030 18.651 1.00 9.10
ATO		3.340 -10.827 18.352 1.00 15.92
ATON		3.783 -11.614 19.575 1.00 15.92
ATON		3.106 -11.780 17.194 1.00 15.92
ATON		2.192 -9.256 19.960 1.00 9.10
ATON		1.707 -9.691 21.003 1.00 15.92
ATON		2.856 -8.106 19.893 1.00 11.07
ATON ATON		3.062 -7.257 21.064 1.00 11.07
ATON		3.959 -6.070 20.705 1.00 16.31 5.377 -6.393 20.229 1.00 16.31
ATON		5.377 -6.393 20.229 1.00 16.31 6.039 -5.149 19.669 1.00 16.31
ATON		6.187 -6.966 21.375 1.00 16.31
ATON		1.729 -6.742 21.595 1.00 11.07
ATON		1.523 -6.650 22.803 1.00 16.31
ATOM		0.827 -6.413 20.677 1.00 13.48
ATOM		-0.494 -5.900 21.015 1.00 13.48
ATOM		-1.185 -5.383 19.752 1.00 15.92
ATOM	1 1259 CG LEU 324	-2.607 -4.837 19.889 1.00 15.92
ATOM	1 1260 CD1 LEU 324	-2.602 -3.547 20.692 1.00 15.92
ATOM	1 1261 CD2 LEU 324	-3.182 -4.598 18.511 1.00 15.92
ATOM	I 1262 C LEU 324	-1.393 -6.924 21.707 1.00 13.48
ATOM	1 1263 O LEU 324	-1.896 -6.678 22.802 1.00 15.92
ATOM	I 1264 N MET 325	-1.593 -8.074 21.072 1.00 11.47
ATOM	I 1265 CA MET 325	-2.458 -9.111 21.631 1.00 11.47
ATOM		-2.959 -10.043 20.520 1.00 22.90
ATOM		-3.689 -9.347 19.375 1.00 22.90
ATOM		-5.052 -8.287 19.908 1.00 22.90
ATOM		-6.284 -9.475 20.353 1.00 22.90
ATOM		-1.814 -9.932 22.752 1.00 11.47
ATOM	1 1271 O MET 325	-1.899 -11.160 22.758 1.00 22.90
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ATOM 1272 N SER 326 -1.193 -9.256 23.711 1.00 30.07 **ATOM** 1273 CA SER 326 -0.543 -9.936 24.826 1.00 30.07 1274 CB SER **ATOM** 326 0.723 -9.175 25.239 1.00 32.79 **ATOM** 1275 OG SER 326 1.283 -9.699 26.433 1.00 32.79 1276 C SER **ATOM** 326 -1.492 -10.061 26.014 1.00 30.07 1277 O **ATOM** SER 326 -2.343 -9.198 26.235 1.00 32.79 **ATOM** 1278 N THR 327 -1.347 -11.143 26.773 1.00 29.08 **ATOM** 1279 CA THR 327 -2.179 -11.368 27.948 1.00 29.08 **ATOM** 1280 CB THR 327 -2.705 -12.817 27.998 1.00 36.96 **ATOM** 1281 OG1 THR 327 -1.612 -13.734 27.856 1.00 36.96 **ATOM** 1282 CG2 THR 327 -3.716 -13.055 26.890 1.00 36.96 **ATOM** 1283 C THR 327 -1.426 -11.049 29.239 1.00 29.08 **ATOM** 1284 O THR 327 -1.930 -11.295 30.333 1.00 36.96 **ATOM** 1285 N **ASP** 328 -0.214 -10.513 29.111 1.00 38.93 **ATOM** 1286 CA ASP 328 0.596 -10.152 30.273 1.00 38.93 **ATOM** 1287 CB ASP 328 2.082 -10.089 29.899 1.00 85.70 **ATOM** 1288 CG ASP 328 2.660 -11.451 29.556 1.00 85.70 ATOM 1289 OD1 ASP 328 3.388 -11.554 28.542 1.00 85.70 **ATOM** 1290 OD2 ASP 328 2.393 -12.418 30.303 1.00 85.70 ATOM 1291 C ASP 328 0.148 -8.810 30.845 1.00 38.93 1292 O **ATOM ASP** 328 0.962 -7.911 31.061 1.00 85.70 1293 N ARG 329 ATOM -1.154 -8.673 31.070 1.00 28.95 **ATOM** 1294 CA ARG 329 -1.716 -7.445 31.608 1.00 28.95 1295 CB ARG 329 **ATOM** -2.390 -6.612 30.509 1.00 38.88 329 **ATOM** 1296 CG ARG -1.449 -5.887 29.554 1.00 38.88 ATOM 1297 CD ARG 329 -1.107 -6.739 28.347 1.00 38.88 1298 NE ARG **ATOM** 329 -0.322 -6.005 27.356 1.00 38.88 **ATOM** 1299 CZ ARG 329 1.006 -5.936 27.351 1.00 38.88 **ATOM** 1300 NH1 ARG 329 1.713 -6.552 28.290 1.00 38.88 **ATOM** 1301 NH2 ARG 329 1.631 -5.270 26.391 1.00 38.88 **ATOM** 1302 C **ARG** 329 -2.745 -7.790 32.672 1.00 28.95 **ATOM** 1303 O **ARG** 329 -3.279 -8.898 32.696 1.00 38.88 **ATOM** 1304 N SER 330 -3.029 -6.829 33.542 1.00 42.07 **ATOM** 1305 CA SER 330 -3.999 -7.025 34.607 1.00 42.07 **ATOM** 1306 CB SER 330 -3.488 -6.399 35.899 1.00 37.35 1307 C SER -5.340 -6.413 34.220 1.00 42.07 **ATOM** 330 **ATOM** 1308 O SER 330 -5.386 -5.382 33.550 1.00 37.35 **ATOM** 1309 N GLY 331 -6.424 -7.085 34.598 1.00 26.57 **ATOM** 1310 CA GLY 331 -7.754 -6.572 34.318 1.00 26.57 **ATOM** 1311 C **GLY** 331 -8.404 -6.915 32.991 1.00 26.57 **ATOM** 1312 O GLY -9.462 -6.371 32.671 1.00 30.06 331 1313 N LEU 332 **ATOM** -7.797 -7.807 32.214 1.00 31.47 **ATOM** 1314 CA LEU 332 -8.374 -8.189 30.928 1.00 31.47 **ATOM** 1315 CB LEU 332 -7.351 -8.933 30.065 1.00 23.83 332 ATOM 1316 CG LEU -6.261 -8.076 29.425 1.00 23.83 **ATOM** 332 1317 CD1 LEU -5.296 -8.960 28.652 1.00 23.83 **ATOM** 1318 CD2 LEU 332 -6.897 -7.041 28.509 1.00 23.83

ATOM	1319 C LEU 332	0.620 0.020 21.001 1.00 21.47
ATOM		-9.630 -9.039 31.091 1.00 31.47
ATOM		-9.665 -9.969 31.895 1.00 23.83
ATOM		-10.659 -8.702 30.321 1.00 27.66
ATOM		-11.927 -9.422 30.351 1.00 27.66
ATOM	·	-13.072 -8.500 29.918 1.00 49.79
ATOM		-13.416 -7.312 30.820 1.00 49.79
ATOM		-14.328 -6.339 30.083 1.00 49.79
ATOM		-14.072 -7.803 32.104 1.00 49.79
ATOM		-11.904 -10.663 29.456 1.00 27.66
ATOM		-12.117 -11.780 29.919 1.00 49.79
ATOM		-11.616 -10.464 28.174 1.00 29.56
ATOM		-11.583 -11.566 27.220 1.00 29.56
ATOM		-12.134 -11.106 25.865 1.00 47.01
		-13.888 -10.657 25.883 1.00 47.01
ATOM ATOM	1333 C CYS 334 1334 O CYS 334	-10.187 -12.161 27.050 1.00 29.56
ATOM		-9.652 -12.202 25.942 1.00 47.01
ATOM	1335 N VAL 335 1336 CA VAL 335	-9.617 -12.655 28.147 1.00 30.69
ATOM	1337 CB VAL 335	-8.280 -13.250 28.132 1.00 30.69
ATOM	1337 CB VAL 335	-7.913 -13.844 29.514 1.00 32.18 -6.517 -14.456 29.480 1.00 32.18
ATOM	1339 CG2 VAL 335	
ATOM	1340 C VAL 335	-7.988 -12.768 30.584 1.00 32.18 -8.120 -14.340 27.068 1.00 30.69
ATOM	1341 O VAL 335	-7.149 -14.337 26.309 1.00 32.18
ATOM	1342 N ASP 336	-9.079 -15.260 27.012 1.00 30.13
ATOM	1343 CA ASP 336	-9.040 -16.360 26.052 1.00 30.13
ATOM	1344 CB ASP 336	-10.218 -17.311 26.284 1.00 63.22
ATOM	1345 CG ASP 336	-10.178 -18.528 25.370 1.00 63.22
ATOM	1346 OD1 ASP 336	-11.119 -18.700 24.565 1.00 63.22
ATOM	1347 OD2 ASP 336	-9.205 -19.311 25.452 1.00 63.22
ATOM	1348 C ASP 336	-9.012 -15.903 24.594 1.00 30.13
ATOM	1349 O ASP 336	-8.156 -16.339 23.823 1.00 63.22
ATOM	1350 N LYS 337	-9.944 -15.027 24.223 1.00 26.63
ATOM	1351 CA LYS 337	-10.024 -14.515 22.856 1.00 26.63
ATOM	1352 CB LYS 337	-11.172 -13.516 22.729 1.00 21.38
ATOM	1353 C LYS 337	-8.706 -13.865 22:438 1.00 26.63
ATOM	1354 O LYS 337	-8.204 -14.110 21.338 1.00 21.38
ATOM	1355 N ILE 338	-8.141 -13.060 23.334 1.00 24.65
ATOM	1356 CA ILE 338	-6.879 -12.376 23.078 1.00 24.65
ATOM	1357 CB ILE 338	-6.543 -11.380 24.215 1.00 20.45
ATOM	1358 CG2 ILE 338	-5.198 -10.719 23.966 1.00 20.45
ATOM	1359 CG1 ILE 338	-7.632 -10.308 24.308 1.00 20.45
ATOM	1360 CD1 ILE 338	-7.479 -9.374 25.486 1.00 20.45
ATOM	1361 C ILE 338	-5.744 -13.388 22.911 1.00 24.65
ATOM	1362 O ILE 338	-4.948 -13.288 21.974 1.00 20.45
ATOM	1363 N GLU 339	-5.700 -14.383 23.795 1.00 35.34
ATOM	1364 CA GLU 339	-4.673 -15.422 23.745 1.00 35.34
ATOM	1365 CB GLU 339	-4.836 -16.388 24.916 1.00 29.51

ATOM 1366 C GLU 339 -4.744 -16.180 22.421 1.00 35.34 **ATOM** 1367 O GLU 339 -3.720 -16.421 21.777 1.00 29.51 **ATOM** 1368 N LYS 340 -5.959 -16.536 22.009 1.00 24.19 1369 CA LYS **ATOM** 340 -6.168 -17.256 20.755 1.00 24.19 **ATOM** 1370 CB LYS 340 -7.627 -17.671 20.624 1.00 23.97 1371 C LYS **ATOM** 340 -5.754 -16.377 19.576 1.00 24.19 1372 O LYS 340 **ATOM** -5.197 -16.860 18.586 1.00 23.97 **ATOM** 1373 N SER 341 -6.000 -15.079 19.708 1.00 16.85 1374 CA SER 341 ATOM -5.651 -14.115 18.676 1.00 16.85 ATOM 1375 CB SER 341 -6.223 -12.744 19.033 1.00 26.59 1376 OG SER **ATOM** 341 -5.852 -11.765 18.080 1.00 26.59 1377 C SER **ATOM** 341 -4.137 -14.026 18.500 1.00 16.85 ATOM 1378 O SER 341 -3.638 -14.042 17.374 1.00 26.59 1379 N GLN **ATOM** 342 -3.406 -13.932 19.608 1.00 17.35 **ATOM** 1380 CA GLN 342 -1.952 -13.845 19.537 1.00 17.35 ATOM 1381 CB GLN 342 -1.337 -13.597 20.913 1.00 30.07 **ATOM** 1382 CG GLN 342 0.140 -13.245 20.832 1.00 30.07 **ATOM** 1383 CD GLN 342 0.811 -13.196 22.182 1.00 30.07 342 **ATOM** 1384 OE1 GLN 0.884 -14.201 22.884 1.00 30.07 1385 NE2 GLN 342 **ATOM** 1.318 -12.030 22.548 1.00 30.07 1386 C GLN 342 **ATOM** -1.368 -15.118 18.944 1.00 17.35 342 ATOM 1387 O GLN -0.405 -15.066 18.178 1.00 30.07 ATOM 1388 N GLU 343 -1.949 -16.260 19.303 1.00 18.35 **ATOM** 1389 CA GLU 343 -1.489 -17.546 18.791 1.00 18.35 1390 CB GLU 343 **ATOM** -2.308 -18.676 19.394 1.00 16.98 1391 C GLU 343 ATOM -1.603 -17.560 17.267 1.00 18.35 1392 O GLU **ATOM** 343 -0.699 -18.026 16.568 1.00 16.98 **ATOM** 1393 N ALA 344 -2.706 -17.017 16.761 1.00 14.83 1394 CA ALA 344 **ATOM** -2.946 -16.948 15.324 1.00 14.83 **ATOM** 1395 CB ALA 344 -4.327 -16.376 15.049 1.00 19.42 **ATOM** 1396 C ALA 344 -1.872 -16.102 14.640 1.00 14.83 **ATOM** 1397 O **ALA** 344 -1.311 -16.507 13.619 1.00 19.42 1398 N TYR 345 ATOM -1.586 -14.934 15.211 1.00 13.10 **ATOM** 1399 CA TYR 345 -0.569 -14.041 14.665 1.00 13.10 **ATOM** 1400 CB TYR 345 -0.573 -12.697 15.393 1.00 2.00 1401 CG TYR 345 -1.670 -11.767 14.938 1.00 2.00 ATOM **ATOM** 1402 CD1 TYR 345 -2.707 -11.409 15.794 1.00 2.00 **ATOM** 1403 CE1 TYR 345 -3.722 -10.562 15.377 1.00 2.00 **ATOM** 1404 CD2 TYR 345 -1.674 -11.248 13.647 1.00 2.00 1405 CE2 TYR **ATOM** 345 -2.683 -10.398 13.219 1.00 2.00 **ATOM** 1406 CZ TYR 345 -3.706 -10.061 14.087 1.00 2.00 1407 OH TYR 345 ATOM -4.722 -9.233 13.669 1.00 2.00 **ATOM** 1408 C **TYR** 345 0.818 -14.666 14.732 1.00 13.10 **ATOM** 1409 O **TYR** 345 1.614 -14.504 13.811 1.00 2.00 1410 N LEU 346 1.101 -15.387 15.813 1.00 12.59 ATOM **ATOM** 1411 CA LEU 346 2.396 -16.041 15.976 1.00 12.59 **ATOM** 1412 CB LEU 346 2.498 -16.715 17.347 1.00 22.61

ATOM 1413 CG LEU 346 2.899 -15.799 18.504 1.00 22.61 **ATOM** 1414 CD1 LEU 346 2.717 -16.511 19.830 1.00 22.61 **ATOM** 1415 CD2 LEU 346 4.341 -15.357 18.324 1.00 22.61 **ATOM** 1416 C LEU 346 2.629 -17.057 14.865 1.00 12.59 **ATOM** 1417 O LEU 346 3.706 -17.099 14.272 1.00 22.61 **ATOM** 1418 N LEU 347 1.612 -17.862 14.574 1.00 18.42 **ATOM** 1419 CA LEU 347 1.706 -18.863 13.517 1.00 18.42 **ATOM** 1420 CB LEU 347 0.471 -19.762 13.512 1.00 23.56 ATOM 1421 CG LEU 347 0.509 -20.965 14.456 1.00 23.56 **ATOM** 1422 CD1 LEU 347 -0.819 -21.702 14.398 1.00 23.56 **ATOM** 1423 CD2 LEU 347 1.659 -21.890 14.068 1.00 23.56 **ATOM** 1424 C LEU 347 1.870 -18.201 12.154 1.00 18.42 **ATOM** 1425 O LEU 347 2.672 -18.651 11.330 1.00 23.56 **ATOM** 1426 N ALA 348 1.099 -17.144 11.917 1.00 12.49 ATOM 1427 CA ALA 348 1.157 -16.403 10.663 1.00 12.49 ATOM 1428 CB ALA 348 0.098 -15.302 10.654 1.00 14.77 **ATOM** 1429 C ALA 348 2.545 -15.798 10.504 1.00 12.49 1430 O **ALA ATOM** 3.154 -15.874 9.436 1.00 14.77 348 1431 N PHE 349 ATOM 3.048 -15.246 11.602 1.00 15.52 **ATOM** 1432 CA PHE 349 4.357 -14.613 11.664 1.00 15.52 **ATOM** 1433 CB PHE 349 4.566 -14.049 13.076 1.00 14.41 **ATOM** 1434 CG PHE 349 5.714 -13.085 13.203 1.00 14.41 **ATOM** 1435 CD1 PHE 349 6.473 -12.712 12.099 1.00 14.41 **ATOM** 1436 CD2 PHE 349 6.027 -12.540 14.443 1.00 14.41 **ATOM** 1437 CE1 PHE 349 7.523 -11.813 12.230 1.00 14.41 ATOM 1438 CE2 PHE 349 7.075 -11.640 14.584 1.00 14.41 **ATOM** 1439 CZ PHE 349 7.825 -11.275 13.475 1.00 14.41 **ATOM** 1440 C PHE 349 5.444 -15.633 11.324 1.00 15.52 ATOM 1441 O PHE 349 6.252 -15.413 10.422 1.00 14.41 **ATOM** 1442 N GLU 350 5.439 -16.760 12.026 1.00 13.20 **ATOM** 1443 CA GLU 350 6.424 -17.811 11.801 1.00 13.20 **ATOM** 1444 CB GLU 350 6.152 -18.995 12.734 1.00 33.43 **ATOM** 1445 CG GLU 350 7.068 -20.193 12.519 1.00 33.43 **ATOM** 1446 CD GLU 350 6.786 -21.331 13.482 1.00 33.43 **ATOM** 1447 OE1 GLU 350 7.746 -22.035 13.857 1.00 33.43 1448 OE2 GLU **ATOM** 350 5.611 -21.525 13.865 1.00 33.43 **ATOM** 1449 C GLU 350 6.409 -18.283 10.352 1.00 13.20 ATOM 1450 O GLU 350 7.449 -18.355 9.694 1.00 33.43 1451 N HIS **ATOM** 351 5.217 -18.573 9.850 1.00 19.10 **ATOM** 1452 CA HIS 351 5.062 -19.051 8.485 1.00 19.10 **ATOM** 1453 CB HIS 351 3.632 -19.536 8.256 1.00 18.97 **ATOM** 1454 CG HIS 351 3.249 -20.700 9.117 1.00 18.97 **ATOM** 1455 CD2 HIS 351 3.987 -21.474 9.948 1.00 18.97 **ATOM** 1456 ND1 HIS 1.960 -21.180 9.194 1.00 18.97 351 1457 CE1 HIS **ATOM** 351 1.918 -22.195 10.039 1.00 18.97 **ATOM** 1458 NE2 HIS 351 3.134 -22.394 10.509 1.00 18.97 **ATOM** 1459 C HIS 351 5.477 -18.011 7.449 1.00 19.10

ATOM 1460 O HIS 351 5.955 -18.366 6.371 1.00 18.97 **ATOM** 1461 N TYR 352 5.304 -16.732 7.767 1.00 9.38 **ATOM** 1462 CA TYR 352 5.711 -15.683 6.843 1.00 9.38 **ATOM** 1463 CB TYR 352 5.168 -14.317 7.257 1.00 16.06 **ATOM** 1464 CG TYR 352 5.539 -13.238 6.268 1.00 16.06 **ATOM** 1465 CD1 TYR 352 5.008 1.00 16.06 4.939 -13.190 **ATOM** 1466 CE1 TYR 352 5.321 -12.242 4.060 1.00 16.06 **ATOM** 1467 CD2 TYR 352 6.531 -12.303 6.562 1.00 16.06 **ATOM** 1468 CE2 TYR 352 6.923 -11.349 5.620 1.00 16.06 1469 CZ TYR **ATOM** 352 6.313 -11.326 4.371 1.00 16.06 **ATOM** 1470 OH TYR 352 6.710 -10.401 3.431 1.00 16.06 **ATOM** 1471 C TYR 352 7.234 -15.639 6.812 1.00 9.38 ATOM 1472 O TYR 352 7.838 -15.475 5.751 1.00 16.06 **ATOM** 1473 N VAL 353 7.851 -15.789 7.980 1.00 15.38 1474 CA VAL **ATOM** 353 9.305 -15.790 8.087 1.00 15.38 1475 CB VAL **ATOM** 353 9.761 -15.945 9.558 1.00 18.40 **ATOM** 1476 CG1 VAL 353 11.262 -16.163 9.633 1.00 18.40 **ATOM** 1477 CG2 VAL 353 9.384 -14.703 10.349 1.00 18.40 **ATOM** 1478 C VAL 353 9.853 -16.938 7.237 1.00 15.38 **ATOM** 1479 O VAL 353 10.850 -16.773 6.525 1.00 18.40 **ATOM** 1480 N **ASN** 354 9.183 -18.086 7.298 1.00 14.74 **ATOM** 1481 CA ASN 354 9.578 -19.259 6.521 1.00 14.74 **ATOM** 1482 CB ASN 354 8.640 -20.435 6.799 1.00 19.97 ATOM 1483 CG ASN 354 8.832 -21.020 8.180 1.00 19.97 **ATOM** 1484 OD1 ASN 354 9.879 -20.848 8.799 1.00 19.97 **ATOM** 1485 ND2 ASN 354 7.826 -21.734 8.664 1.00 19.97 **ATOM** 1486 C ASN 354 9.550 -18.939 5.034 1.00 14.74 **ASN ATOM** 1487 O 354 .10.452 -19.319 4.290 1.00 19.97 **ATOM** 1488 N HIS 355 8.507 -18.230 4.613 1.00 13.03 **ATOM** 1489 CA HIS 355 3.220 1.00 13.03 8.329 -17.837 1490 CB HIS **ATOM** 355 6.960 -17.164 3.042 1.00 24.39 **ATOM** 1491 CG HIS 355 6.753 -16.541 1.695 1.00 24.39 **ATOM** 1492 CD2 HIS 355 7.195 -15.370 1.176 1.00 24.39 **ATOM** 1493 ND1 HIS 355 6.009 -17.138 0.701 1.00 24.39 ATOM 1494 CE1 HIS 355 6.005 -16.368 -0.372 1.00 24.39 **ATOM** 1495 NE2 HIS 355 6.720 -15.289 -0.107 1.00 24.39 **ATOM** 1496 C HIS 355 9.434 -16.894 2.758 1.00 13.03 HIS 1497 O 355 **ATOM** 9.834 -16.920 1.595 1.00 24.39 **ATOM** 1498 N **ARG** 356 9.878 -16.027 3.660 1.00 19.55 1499 CA ARG **ATOM** 356 10.920 -15.054 3.358 1.00 19.55 1500 CB ARG 356 ATOM 10.970 -14.001 4.460 1.00 22.01 **ATOM** 1501 CG ARG 356 9.772 -13.081 4.454 1.00 22.01 **ATOM** 1502 CD ARG 356 10.097 -11.784 3.750 1.00 22.01 **ATOM** 1503 NE ARG 356 10.932 -10.934 4.592 1.00 22.01 **ATOM** 1504 CZ ARG 356 11.822 -10.059 4.137 1.00 22.01 1505 NH1 ARG **ATOM** 356 12.010 -9.907 2.833 1.00 22.01 ATOM 1506 NH2 ARG 356 12.519 -9.325 4.992 1.00 22.01

ATOM	1507 C ARG 356	12.297 -15.675 3.158 1.00 19.55
ATOM	1508 O ARG 356	13.127 -15.126 2.434 1.00 22.01
ATOM	1509 N LYS 357	12.547 -16.788 3.841 1.00 23.18
ATOM	1510 CA LYS 357	13.815 -17.504 3.739 1.00 23.18
ATOM	1511 CB LYS 357	13.879 -18.273 2.415 1.00 42.91
ATOM	1512 CG LYS 357	12.750 -19.277 2.274 1.00 42.91
ATOM		12.773 -20.021 0.960 1.00 42.91
ATOM		11.619 -21.011 0.913 1.00 42.91
ATOM		11.629 -21.845 -0.316 1.00 42.91
ATOM		15.047 -16.619 3.918 1.00 23.18
ATOM	1517 O LYS 357	15.816 -16.396 2.982 1.00 42.91
ATOM		15.228 -16.122 5.137 1.00 32.39
ATOM	1519 CA HIS 358	16.367 -15.272 5.460 1.00 32.39
ATOM	1520 CB HIS 358	16.181 -14.626 6.835 1.00 26.77
ATOM	1521 CG HIS 358	15.232 -13.468 6.841 1.00 26.77
ATOM	1522 CD2 HIS 358	15.452 -12.138 6.709 1.00 26.77
ATOM	1522 CD2 HIS 358	
ATOM	1524 CE1 HIS 358	13.875 -13.615 7.028 1.00 26.77 13.300 -12.426 7.012 1.00 26.77
ATOM	1525 NE2 HIS 358	14.234 -11.513 6.821 1.00 26.77
ATOM	1526 C HIS 358	.,
ATOM	1527 O HIS 358	17.633 -16.115
ATOM	1528 N ASN 359	18.728 -15.561 4.972 1.00 41.97
ATOM	1529 CA ASN 359	20.000 -16.273 4.959 1.00 41.97
ATOM	1530 CB ASN 359	20.909 -15.716 3.863 1.00 46.84
ATOM	1531 C ASN 359	20.663 -16.134 6.331 1.00 41.97
ATOM	1532 O ASN 359	21.821 -15.731 6.436 1.00 46.84
ATOM	1533 N ILE 360	19.908 -16.450 7.379 1.00 35.72
ATOM	1534 CA ILE 360	20.394 -16.359 8.753 1.00 35.72
ATOM	1535 CB ILE 360	19.819 -15.113 9.480 1.00 36.14
ATOM	1536 CG2 ILE 360	20.327 -15.050 10.918 1.00 36.14
ATOM	1537 CG1 ILE 360	20.204 -13.833 8.734 1.00 36.14
ATOM	1538 CD1 ILE 360	19.526 -12.591 9.265 1.00 36.14
ATOM	1539 C ILE 360	19.935 -17.611 9.493 1.00 35.72
ATOM	1540 O ILE 360	18.748 -17.953 9.479 1.00 36.14
ATOM	1541 N PRO 361	20.877 -18.338 10:109 1.00 31.56
ATOM	1542 CD PRO 361	22.334 -18.114 10.100 1.00 33.50
ATOM	1543 CA PRO 361	20.532 -19.556 10.847 1.00 31.56
ATOM	1544 CB PRO 361	21.901 -20.163 11.161 1.00 33.50
ATOM	1545 CG PRO 361	22.801 -18.967 11.249 1.00 33.50
ATOM	1546 C PRO 361	19.743 -19.256 12.121 1.00 31.56
ATOM	1547 O PRO 361	20.080 -18.338 12.867 1.00 33.50
ATOM	1548 N HIS 362	18.688 -20.034 12.355 1.00 18.84
ATOM	1549 CA HIS 362	17.840 -19.887 13.541 1.00 18.84
ATOM	1550 CB HIS 362	18.656 -20.151 14.812 1.00 31.38
ATOM	1551 CG HIS 362	19.540 -21.357 14.731 1.00 31.38
ATOM	1552 CD2 HIS 362	19.250 -22.667 14.537 1.00 31.38
ATOM	1553 ND1 HIS 362	20.910 -21.286 14.860 1.00 31.38
		20.510 21.200 14.000 1.00 51.50

1554 CE1 HIS ATOM 362 21.427 -22.497 14.754 1.00 31.38 **ATOM** 1555 NE2 HIS 362 20.439 -23.353 14.558 1.00 31.38 **ATOM** 1556 C HIS 362 17.189 -18.506 13.628 1.00 18.84 **ATOM** 1557 O HIS 362 16.980 -17.979 14.723 1.00 31.38 **ATOM** 1558 N PHE 363 16.825 -17.950 12.476 1.00 18.69 **ATOM** 1559 CA PHE 363 16.209 -16.630 12.408 1.00 18.69 **ATOM** 1560 CB PHE 363 15.825 -16.302 10.962 1.00 19.25 **ATOM** 1561 CG PHE 363 15.339 -14.894 10.765 1.00 19.25 **ATOM** 1562 CD1 PHE 363 16.239 -13.862 10.530 1.00 19.25 **ATOM** 1563 CD2 PHE 363 13.981 -14.598 10.819 1.00 19.25 **ATOM** 1564 CE1 PHE 363 15.794 -12.556 10.351 1.00 19.25 **ATOM** 1565 CE2 PHE 363 13.527 -13.296 10.642 1.00 19.25 **ATOM** 1566 CZ PHE 363 14.435 -12.273 10.407 1.00 19.25 **ATOM** 1567 C PHE 363 14.995 -16.461 13.323 1.00 18.69 **ATOM** 1568 O PHE 363 14.955 -15.540 14.138 1.00 19.25 **ATOM** 1569 N TRP 364 14.016 -17.351 13.191 1.00 16.46 **ATOM** 1570 CA TRP 364 12.797 -17.280 13.995 1.00 16.46 **ATOM** 1571 CB TRP 364 -11.882 -18.482 13.706 1.00 17.81 **ATOM** 1572 CG TRP 364 10.588 -18.488 14.481 1.00 17.81 **ATOM** 1573 CD2 TRP 364 9.586 -17.458 14.504 1.00 17.81 **ATOM** 1574 CE2 TRP 364 8.547 -17.905 15.350 1.00 17.81 **ATOM** 1575 CE3 TRP 364 9.467 -16.202 13.894 1.00 17.81 **ATOM** 1576 CD1 TRP 364 10.126 -19.486 15.290 1.00 17.81 **ATOM** 1577 NE1 TRP 364 8.902 -19.144 15.814 1.00 17.81 **ATOM** 1578 CZ2 TRP 364 7.403 -17.142 15.602 1.00 17.81 **ATOM** 1579 CZ3 TRP 364 8.329 -15.444 14.145 1.00 17.81 **ATOM** 1580 CH2 TRP 364 7.312 -15.919 14.992 1.00 17.81 **ATOM** 1581 C TRP 364 13.046 -17.114 15.500 1.00 16.46 ATOM 1582 O TRP 364 12.595 -16.133 16.087 1.00 17.81 **ATOM** 1583 N PRO 365 13.779 -18.051 16.137 1.00 18.31 **ATOM** 1584 CD PRO 365 14.342 -19.314 15.625 1.00 25.61 **ATOM** 1585 CA PRO 365 14.038 -17.920 17.577 1.00 18.31 **ATOM** 1586 CB PRO 365 14.939 -19.118 17.874 1.00 25.61 **ATOM** 1587 CG PRO 365 14.500 -20.130 16.882 1.00 25.61 **ATOM** 1588 C **PRO** 365 14.732 -16.606 17.933 1.00 18.31 **ATOM** 1589 O **PRO** 365 14.387 -15.963 18.926 1.00 25.61 1590 N LYS **ATOM** 366 15.699 -16.207 17.112 1.00 25.16 **ATOM** 1591 CA LYS 366 16.439 -14.968 17.338 1.00 25.16 1592 CB LYS **ATOM** 366 17.537 -14.805 16.289 1.00 40.51 ATOM 1593 CG LYS 366 18.679 -15.792 16.417 1.00 40.51 **ATOM** 1594 CD LYS 366 19.664 -15.607 15.278 1.00 40.51 **ATOM** 1595 CE LYS 366 20.884 -16.492 15.440 1.00 40.51 **ATOM** 1596 NZ LYS 366 21.800 -16.360 14.275 1.00 40.51 **ATOM** 1597 C LYS 366 15.521 -13.747 17.317 1.00 25.16 **ATOM** 1598 O LYS 366 15.593 -12.893 18.202 1.00 40.51 **ATOM** 1599 N LEU 367 14.661 -13.666 16.307 1.00 25.30 **ATOM** 1600 CA LEU 367 13.729 -12.551 16.184 1.00 25.30

ATOM 1601 CB LEU 367 12.989 -12.620 14.845 1.00 27.80 **ATOM** 1602 CG LEU 367 11.964 -11.519 14.561 1.00 27.80 **ATOM** 1603 CD1 LEU 367 12.621 -10.147 14.679 1.00 27.80 **ATOM** 1604 CD2 LEU 367 11.367 -11.724 13.175 1.00 27.80 1605 C LEU **ATOM** 367 12.730 -12.596 17.332 1.00 25.30 ATOM 1606 O' LEU 367 12.337 -11.563 17.877 1.00 27.80 **ATOM** 1607 N LEU 368 12.345 -13.807 17.712 1.00 26.12 **ATOM** 1608 CA LEU 368 11.396 -14.019 18.793 1.00 26.12 ATOM 1609 CB LEU 368 11.105 -15.515 18.919 1.00 33.27 ATOM 1610 CG LEU 368 9.696 -15.976 19.289 1.00 33.27 **ATOM** 1611 CD1 LEU 368 8.640 -15.182 18.529 1.00 33.27 **ATOM** 1612 CD2 LEU 368 9.582 -17.460 18.976 1.00 33.27 **ATOM** 1613 C LEU 368 11.973 -13.466 20.096 1.00 26.12 **ATOM** LEU 1614 O 368 11.249 -12.920 20.930 1.00 33.27 **ATOM** 1615 N MET 369 13.289 -13.571 20.244 1.00 24.39 **ATOM** 1616 CA MET 369 13.971 -13.076 21.432 1.00 24.39 ATOM 1617 CB MET 369 15.382 -13.656 21.511 1.00 47.44 15.407 -15.096 22.009 1.00 47.44 **ATOM** 1618 CG MET 369 **ATOM** 1619 SD MET 369 16.850 -16.029 21.464 1.00 47.44 **ATOM** 1620 CE MET 369 18.186 -15.114 22.246 1.00 47.44 **ATOM** 1621 C MET 369 13.996 -11.552 21.491 1.00 24.39 **ATOM** 1622 O **MET** 369 14.212 -10.971 22.557 1.00 47.44 **ATOM** 1623 N LYS 370 13.749 -10.904 20.354 1.00 27.31 1624 CA LYS **ATOM** 370 13.713 -9.445 20.297 1.00 27.31 **ATOM** 1625 CB LYS 370 13.739 -8.951 18.847 1.00 28.20 **ATOM** 1626 CG LYS 370 15.004 -9.312 18.090 1.00 28.20 **ATOM** 1627 CD LYS 370 16.231 -8.810 18.824 1.00 28.20 **ATOM** 1628 CE LYS 370 17.512 -9.244 18.142 1.00 28.20 **ATOM** 1629 NZ LYS 370 18.696 -8.851 18.952 1.00 28.20 **ATOM** 1630 C LYS 12.453 -8.945 21.002 1.00 27.31 370 **ATOM** 1631 O LYS 370 12.424 -7.835 21.535 1.00 28.20 371 **ATOM** 1632 N VAL 11.413 -9.776 21.009 1.00 26.41 **ATOM** 1633 CA VAL 371 10.157 -9.432 21.668 1.00 26.41 9.109 -10.561 21.512 1.00 25.61 **ATOM** 1634 CB VAL 371 **ATOM** 1635 CG1 VAL 371 7.825 -10.205 22.245 1.00 25.61 371 ATOM 1636 CG2 VAL 8.819 -10.805 20.044 1.00 25.61 **ATOM** VAL 1637 C 371 10.450 -9.205 23.151 1.00 26.41 1638 O VAL 371 9.962 -8.248 23.752 1.00 25.61 **ATOM ATOM** 1639 N THR 372 11.294 -10.065 23.713 1.00 26.28 **ATOM** 1640 CA THR 372 11.683 -9.972 25.116 1.00 26.28 12.656 -11.109 25.500 1.00 28.14 372 **ATOM** 1641 CB THR 372 **ATOM** 1642 OG1 THR 12.025 -12.377 25.275 1.00 28.14 **ATOM** 1643 CG2 THR 372 13.055 -11.001 26.965 1.00 28.14 **ATOM** 1644 C THR 372 12.358 -8.624 25.372 1.00 26.28 ATOM 1645 O THR 372 12.047 -7.937 26.350 1.00 28.14 **ATOM** 1646 N ASP 373 13.269 -8.247 24.478 1.00 15.09 13.977 -6.979 24.588 1.00 15.09 **ATOM** 1647 CA ASP 373

ATOM 1648 CB ASP 373 14.976 -6.822 23.435 1.00 37.94 **ATOM** 1649 CG ASP 373 16.065 -7.893 23.445 1.00 37.94 **ATOM** 1650 OD1 ASP 373 16.248 -8.571 24.483 1.00 37.94 **ATOM** 1651 OD2 ASP 373 16.750 -8.052 22.410 1.00 37.94 1652 C **ATOM ASP** 373 12.969 -5.833 24.577 1.00 15.09 **ATOM** 1653 O ASP 373 13.040 -4.928 25.407 1.00 37.94 **ATOM** 1654 N LEU 374 12.008 -5.901 23.659 1.00 17.04 **ATOM** 1655 CA LEU 374 10.974 -4.880 23.549 1.00 17.04 **ATOM** 1656 CB LEU 374 10.071 -5.155 22.344 1.00 20.58 **ATOM** 1657 CG LEU 374 10.624 -4.720 20.985 1.00 20.58 **ATOM** 1658 CD1 LEU 374 9.826 -5.352 19.862 1.00 20.58 **ATOM** 1659 CD2 LEU 374 10.599 -3.202 20.882 1.00 20.58 1660 C **ATOM** LEU 374 10.145 -4.786 24.825 1.00 17.04 **ATOM** 1661 O LEU 374 9.783 -3.688 25.256 1.00 20.58 ATOM 1662 N **ARG** 375 9.850 -5.935 25.430 1.00 20.46 **ATOM** 1663 CA ARG 375 9.080 -5.977 26.673 1.00 20.46 **ATOM** 1664 CB ARG 375 8.873 -7.422 27.140 1.00 55.89 ATOM 1665 CG ARG 375 8.180 -8.354 26.152 1.00 55.89 ATOM 1666 CD ARG 375 6.692 -8.084 26.027 1.00 55.89 **ATOM** 1667 NE ARG 375 5.943 -9.338 25.968 1.00 55.89 **ATOM** 1668 CZ ARG 375 5.054 -9.654 25.028 1.00 55.89 ATOM 1669 NH1 ARG 375 4.782 -8.808 24.040 1.00 55.89 **ATOM** 1670 NH2 ARG 375 4.438 -10.829 25.073 1.00 55.89 ATOM 1671 C ARG 375 9.874 -5.221 27.735 1.00 20.46 **ATOM** 1672 O **ARG** 375 9.328 -4.391 28.463 1.00 55.89 **ATOM** 1673 N **MET** 376 11.174 -5.502 27.794 1.00 20.10 **ATOM** 1674 CA MET 376 12.076 -4.863 28.744 1.00 20.10 ATOM 1675 CB MET 376 13.493 -5.417 28.580 1.00 63.73 **ATOM** 1676 CG MET 376 13.956 -6.310 29.722 1.00 63.73 **ATOM** 1677 SD MET 376 14.494 -5.373 31.182 1.00 63.73 **ATOM** 1678 CE MET 376 12.934 -5.151 32.087 1.00 63.73 **ATOM** 1679 C **MET** 376 12.081 -3.347 28.566 1.00 20.10 **ATOM** 1680 O **MET** 376 11.973 -2.602 29.539 1.00 63.73 **ATOM** 1681 N ILE 377 12.194 -2.896 27.321 1.00 30.02 **ATOM** 1682 CA ILE 377 12.198 -1.469 27.014 1.00 30.02 **ATOM** 1683 CB ILE 377 12.329 -1.228 25.488 1.00 19.31 **ATOM** 1684 CG2 ILE 377 12.088 0.242 25.152 1.00 19.31 **ATOM** 1685 CG1 ILE 377 13.711 -1.685 25.011 1.00 19.31 **ATOM** 1686 CD1 ILE 377 13.906 -1.634 23.507 1.00 19.31 **ATOM** 1687 C ILE 377 10.915 -0.821 27.542 1.00 30.02 **ATOM** 1688 O ILE 377 10.962 0.216 28.211 1.00 19.31 **ATOM** 1689 N **GLY** 378 9.779 -1.455 27.266 1.00 21.85 **ATOM** 1690 CA GLY 378 8.505 -0.936 27.729 1.00 21.85 **GLY ATOM** 1691 C 378 8.459 -0.821 29.243 1.00 21.85 **ATOM** 1692 O GLY 378 7.990 0.185 29.779 1.00 34.01 8.967 -1.842 29.928 1.00 31.30 **ATOM** 1693 N ALA 379 **ATOM** 8.996 -1.870 31.388 1.00 31.30 1694 CA ALA 379

ATOM 1695 CB ALA 379 9.471 -3.231 31.880 1.00 30.06 **ATOM** 1696 C **ALA** 379 9.895 -0.763 31.938 1.00 31.30 **ATOM** 1697 O **ALA** 379 9.482 0.002 32.810 1.00 30.06 **ATOM** 1698 N **CYS** 380 11.117 -0.677 31.418 1.00 28.61 1699 CA CYS **ATOM** 380 12.067 0.349 31.841 1.00 28.61 **ATOM** 1700 CB CYS 380 13.360 0.268 31.025 1.00 60.26 **ATOM** 1701 SG CYS 380 14.499 -1.067 31.470 1.00 60.26 **ATOM** 1702 C **CYS** 380 11.449 1.730 31.658 1.00 28.61 **ATOM** 1703 O **CYS** 380 11.516 2.573 32.554 1.00 60.26 **ATOM** 1704 N HIS 381 10.840 1.957 30.498 1.00 30.42 **ATOM** 1705 CA HIS 381 10.212 3.243 30.216 1.00 30.42 ATOM 1706 CB HIS 381 9.696 3.306 28.779 1.00 16.49 **ATOM** 1707 CG HIS 381 8.942 4.562 28.472 1.00 16.49 **ATOM** 1708 CD2 HIS 381 9.370 5.805 28.151 1.00 16.49 **ATOM** 1709 ND1 HIS 381 7.566 4.633 28.524 1.00 16.49 **ATOM** 1710 CE1 HIS 381 7.180 5.866 28.251 1.00 16.49 ATOM 1711 NE2 HIS 381 8.255 6.596 28.021 1.00 16.49 **ATOM** 1712 C HIS 381 9.073 3.539 31.182 1.00 30.42 **ATOM** 1713 O HIS 381 8.856 4.690 31.552 1.00 16.49 **ATOM** 1714 N ALA 382 8.330 2.506 31.564 1.00 22.89 **ATOM** 1715 CA ALA 382 7.218 2.666 32.493 1.00 22.89 **ATOM** 1716 CB ALA 382 6.520 1.336 32.708 1.00 34.50 **ATOM** 1717 C ALA 382 7.738 3.213 33.819 1.00 22.89 **ATOM** 1718 O **ALA** 382 7.219 4.200 34.343 1.00 34.50 **ATOM** 1719 N SER 383 8.789 2.586 34.336 1.00 26.39 **ATOM** 1720 CA SER 383 9.400 3.006 35.591 1.00 26.39 **ATOM** 1721 CB SER 383 10.510 2.030 35.985 1.00 52.94 **ATOM** 1722 OG SER 383 10.015 0.702 36.046 1.00 52.94 **ATOM** 1723 C SER 383 9.966 4.418 35.470 1.00 26.39 **ATOM** 1724 O. SER 383 9.772 5.253 36.357 1.00 52.94 **ATOM** 1725 N **ARG** 384 10.662 4.683 34.368 1.00 30.36 **ATOM** 1726 CA ARG 384 11.249 5.995 34.134 1.00 30.36 **ATOM** 1727 CB ARG 384 12.116 5.977 32.874 1.00 37.39 ATOM 1728 CG ARG 384 12.601 7.344 32.431 1.00 37.39 **ATOM** 1729 CD ARG 384 14.070 7.321 32.060 1.00 37.39 **ATOM** 1730 NE ARG 384 14.935 7.597 33.204 1.00 37.39 **ATOM** 1731 CZ ARG 384 15.750 8.646 33.291 1.00 37.39 **ATOM** 1732 NH1 ARG 384 15.824 9.529 32.303 1.00 37.39 1733 NH2 ARG **ATOM** 384 16.488 8.819 34.376 1.00 37.39 **ATOM** 1734 C **ARG** 384 10.169 7.067 34.030 1.00 30.36 **ATOM** 1735 O **ARG** 384 10.301 8.144 34.616 1.00 37.39 1736 N PHE **ATOM** 385 9.078 6.749 33.338 1.00 24.47 **ATOM** 1737 CA PHE 385 7.980 7.693 33.171 1.00 24.47 **ATOM** 1738 CB PHE 385 6.859 7.092 32.319 1.00 28.70 ATOM 1739 CG PHE 385 5.710 8.036 32.075 1.00 28.70 **ATOM** 1740 CD1 PHE 385 5.795 9.017 31.092 1.00 28.70 **ATOM** 1741 CD2 PHE 385 4.549 7.954 32.836 1.00 28.70

ATOM 1742 CE1 PHE 385 4.740 9.903 30.874 1.00 28.70 **ATOM** 1743 CE2 PHE 385 3.491 8.835 32.624 1.00 28.70 **ATOM** 1744 CZ PHE 385 3.587 9.812 31.641 1.00 28.70 **ATOM** 1745 C PHE 385 7.436 8.097 34.533 1.00 24.47 **ATOM** 1746 O PHE 385 9.285 34.805 1.00 28.70 7.250 **ATOM** 1747 N LEU 386 7.208 7.107 35.391 1.00 31.13 **ATOM** 1748 CA LEU 386 6.690 7.352 36.734 1.00 31.13 **ATOM** 1749 CB LEU 6.596 386 6.044 37.513 1.00 39.10 **ATOM** 1750 C LEU 386 7.577 8.348 37.474 1.00 31.13 **ATOM** 1751 O LEU 386 7.085 9.201 38.217 1.00 39.10 HIS 8.884 ATOM 1752 N 387 8.254 37.243 1.00 36.46 9.837 9.152 37.881 1.00 36.46 **ATOM** 1753 CA HIS 387 1754 CB HIS **ATOM** 387 11.258 8.589 37.794 1.00 62.78 **ATOM** 1755 CG HIS 387 11.459 7.338 38.590 1.00 62.78 **ATOM** 1756 CD2 HIS 387 10.601 6.614 39.346 1.00 62.78 **ATOM** 1757 ND1 HIS 387 12.675 6.689 38.663 1.00 62.78 **ATOM** 1758 CE1 HIS 387 12.554 5.620 39.431 1.00 62.78 ATOM 1759 NE2 HIS 387 11.309 5.550 39.856 1.00 62.78 ATOM 1760 C HIS 387 9.778 10.544 37.266 1.00 36.46 **ATOM** 1761 O HIS 387 9.885 11.543 37.979 1.00 62.78 **ATOM** 1762 N MET 388 9.587 10.612 35.950 1.00 33.41 **ATOM** 1763 CA MET 388 9.505 11.894 35.258 1.00 33.41 **ATOM** 1764 CB MET 388 9.269 11.703 33.755 1.00 42.63 **ATOM** 1765 CG MET 388 10.456 11.144 32.982 1.00 42.63 **ATOM** 1766 SD MET 388 10.253 11.325 31.192 1.00 42.63 **ATOM** 1767 CE MET 388 9.501 9.772 30.748 1.00 42.63 1768 C 388 **ATOM MET** 8.385 12.746 35.849 1.00 33.41 1769 O **MET** 388 ATOM 8.573 13.934 36.103 1.00 42.63 1770 N LYS 389 ATOM 7.235 12.126 36.092 1.00 39.26 **ATOM** 1771 CA LYS 389 6.082 12.825 36.659 1.00 39.26 1772 CB LYS 389 **ATOM** 4.867 11.900 36.719 1.00 52.87 **ATOM** 1773 CG LYS 389 4.237 11.594 35.379 1.00 52.87 **ATOM** 1774 CD LYS 389 3.048 10.667 35.553 1.00 52.87 **ATOM** 1775 CE LYS 389 3.482 9.327 36.125 1.00 52.87 389 **ATOM** 1776 NZ LYS 2.335 8.407 36.326 1.00 52.87 **ATOM** 1777 C LYS 389 6.363 13.360 38.056 1.00 39.26 **ATOM** 1778 O LYS 389 5.837 14.404 38.452 1.00 52.87 VAL 390 ATOM 1779 N 7.156 12.614 38.818 1.00 44.18 1780 CA VAL 390 **ATOM** 7.508 13.016 40.172 1.00 44.18 390 1781 CB VAL 8.299 11.898 40.905 1.00 50.50 **ATOM** 1782 CG1 VAL 390 ATOM 8.718 12.362 42.293 1.00 50.50 390 **ATOM** 1783 CG2 VAL 7.455 10.640 41.012 1.00 50.50 **ATOM** 1784 C VAL 390 8.352 14.288 40.145 1.00 44.18 **ATOM** 1785 O VAL 390 8.144 15.198 40.948 1.00 50.50 **ATOM** 1786 N. GLU 391 9.261 14.368 39.179 1.00 38.64 **ATOM** 1787 CA GLU 391 10.161 15.509 39.056 1.00 38.64 1788 CB GLU 391 11.483 15.060 38.424 1.00 64.18 **ATOM**

1789 CG GLU ATOM 12.065 13.766 39.009 1.00 64.18 391 **ATOM** 1790 CD GLU 391 12.662 13.922 40.405 1.00 64.18 **ATOM** 1791 OE1 GLU 391 12.190 14.773 41.192 1.00 64.18 1792 OE2 GLU **ATOM** 391 13.611 13.173 40.721 1.00 64.18 **ATOM** 1793 C GLU 391 9.623 16.737 38.314 1.00 38.64 1794 O' GLU **ATOM** 391 9.656 17.850 38.849 1.00 64.18 1795 N CYS **ATOM** 392 9.125 16.539 37.096 1.00 37.24 **ATOM** 1796 CA CYS 392 8.611 17.635 36.271 1.00 37.24 **ATOM** 1797 CB CYS 392 8.879 17.345 34.784 1.00 30.64 **ATOM** 1798 SG CYS 392 10.634 17.137 34.283 1.00 30.64 **ATOM** 1799 C **CYS** 392 7.110 17.882 36.496 1.00 37.24 **ATOM** 1800 O **CYS** 392 6.403 17.011 37.006 1.00 30.64 **ATOM** 1801 N PRO 393 6.625 19.107 36.199 1.00 40.56 **ATOM** 1802 CD PRO 393 7.444 20.297 35.904 1.00 33.41 **ATOM** 1803 CA PRO 393 5.209 19.473 36.358 1.00 40.56 **ATOM** 1804 CB PRO 393 5.253 21.001 36.404 1.00 33.41 **ATOM** 1805 CG PRO 393 6.409 21.332 35.527 1.00 33.41 **ATOM** 1806 C PRO 393 4.330 18.975 35.207 1.00 40.56 **ATOM** 1807 O **PRO** 393 4.776 18.907 34.057 1.00 33.41 **ATOM** 1808 N THR 394 3.067 18.691 35.516 1.00 41.91 **ATOM** 1809 CA THR 394 2.101 18.186 34.540 1.00 41.91 **ATOM** 1810 CB THR 394 0.691 18.075 35.156 1.00 62.04 **ATOM** 1811 OG1 THR 394 0.706 18.582 36.497 1.00 62.04 ATOM 1812 CG2 THR 394 0.232 16.626 35.168 1.00 62.04 ATOM 1813 C THR 394 1.995 18.984 33.242 1.00 41.91 **ATOM** 1814 O THR 394 1.758 18.411 32.181 1.00 62.04 **ATOM** 1815 N GLU 395 2.191 20.297 33.327 1.00 43.92 ATOM 1816 CA GLU 395 2.104 21.176 32.160 1.00 43.92 **ATOM** 1817 CB GLU 395 2.313 22.626 32.585 1.00 34.22 **ATOM** 1818 C 395 GLU 3.071 20.814 31.031 1.00 43.92 **ATOM** 1819 O **GLU** 395 2.887 21.243 29.891 1.00 34.22 **ATOM** 1820 N LEU 396 4.104 20.041 31.350 1.00 34.92 **ATOM** 1821 CA LEU 396 5.096 19.634 30.359 1.00 34.92 ATOM 1822 CB LEU 396 6.473 19.495 31.017 1.00 35.81 **ATOM** 1823 CG LEU 396 7.074 20.747 31.662 1.00 35.81 **ATOM** 1824 CD1 LEU 396 8.427 20.410 32.263 1.00 35.81 **ATOM** 1825 CD2 LEU 396 7.209 21.857 30.629 1.00 35.81 **ATOM** 1826 C LEU 396 4.731 18.324 29.661 1.00 34.92 1827 O ATOM LEU 396 5.343 17.954 28.659 1.00 35.81 **ATOM** 1828 N PHE 397 3.734 17.627 30.197 1.00 35.28 **ATOM** 1829 CA PHE 397 3.302 16.352 29.640 1.00 35.28 **ATOM** 1830 CB PHE 397 3.059 15.341 30.764 1.00 27.13 **ATOM** 1831 CG PHE 397 4.285 15.004 31.561 1.00 27.13 397 **ATOM** 1832 CD1 PHE 4.700 15.824 32.604 1.00 27.13 **ATOM** 1833 CD2 PHE 397 5.021 13.860 31.273 1.00 27.13 1834 CE1 PHE 397 **ATOM** 5.831 15.510 33.349 1.00 27.13 1835 CE2 PHE 397 **ATOM** 6.155 13.537 32.013 1.00 27.13

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ATOM	1836 CZ PHE 397	6.561 14.364 33.052 1.00 27.13
ATOM		2.027 16.474 28.812 1.00 35.28
ATOM		0.977 16.861 29.331 1.00 27.13
ATOM		2.102 16.164 27.505 1.00 26.41
ATOM		3.305 15.850 26.713 1.00 19.32
ATOM		0.917 16.247 26.647 1.00 26.41
ATOM		1.439 15.752 25.300 1.00 19.32
ATOM	•	2.867 16.193 25.312 1.00 19.32
ATOM		-0.157 15.313 27.206 1.00 26.41
ATOM		0.160 14.232 27.710 1.00 19.32
ATOM	1846 N PRO 399	-1.439 15.702 27.104 1.00 25.12
ATOM	1847 CD PRO 399	-1.935 16.929 26.454 1.00 24.32
ATOM		-2.554 14.894 27.612 1.00 25.12
ATOM ATOM		-3.777 15.594 27.022 1.00 24.32
ATOM	1850 CG PRO 399 1851 C PRO 399	-3.349 17.026 26.974 1.00 24.32 2.502 13.416 27.222 1.00 25.12
ATOM	1852 O PRO 399	-2.502 13.416 27.222 1.00 25.12 -2.599 12.540 28.085 1.00 24.32
ATOM	1853 N LEU 400	-2.322 13.139 25.933 1.00 23.10
ATOM	1854 CA LEU 400	-2.265 11.759 25.454 1.00 23.10
ATOM	1855 CB LEU 400	-2.230 11.720 23.923 1.00 22.35
ATOM	1856 CG LEU 400	-2.485 10.354 23.276 1.00 22.35
ATOM	1857 CD1 LEU 400	-3.792 9.765 23.792 1.00 22.35
ATOM	1858 CD2 LEU 400	-2.523 10.494 21.763 1.00 22.35
ATOM	1859 C LEU 400	-1.066 11.012 26.032 1.00 23.10
ATOM	1860 O LEU 400	-1.160 9.825 26.345 1.00 22.35
ATOM	1861 N PHE 401	0.044 11.723 26.202 1.00 13.85
ATOM	1862 CA PHE 401	1.269 11.150 26.755 1.00 13.85
ATOM	1863 CB PHE 401	2.374 12.213 26.753 1.00 26.97
ATOM	1864 CG PHE 401	3.729 11.702 27.164 1.00 26.97
ATOM	1865 CD1 PHE 401	4.189 10.461 26.732 1.00 26.97
ATOM	1866 CD2 PHE 401	4.561 12.481 27.963 1.00 26.97
ATOM	1867 CE1 PHE 401	5.459 10.005 27.091 1.00 26.97
ATOM	1868 CE2 PHE 401	5.830 12.035 28.327 1.00 26.97
ATOM	1869 CZ PHE 401	6.280 10.795 27.889 1.00 26.97
ATOM	1870 C PHE 401	0.993 10.659 28.179 1.00 13.85
ATOM ATOM	1871 O PHE 401 1872 N LEU 402	1.393 9.558 28.555 1.00 26.97 0.274 11.473 28.947 1.00 25.21
ATOM	1873 CA LEU 402	-0.080 11.145 30.325 1.00 25.21
ATOM	1874 CB LEU 402	-0.640 12.380 31.035 1.00 29.34
ATOM	1875 CG LEU 402	0.334 13.411 31.600 1.00 29.34
ATOM	1876 CD1 LEU 402	-0.430 14.658 32.018 1.00 29.34
ATOM	1877 CD2 LEU 402	1.090 12.814 32.775 1.00 29.34
ATOM	1878 C LEU 402	-1.109 10.025 30.425 1.00 25.21
ATOM	1879 O LEU 402	-1.034 9.189 31.320 1.00 29.34
ATOM	1880 N GLU 403	-2.090 10.043 29.529 1.00 23.54
ATOM	1881 CA GLU 403	-3.159 9.046 29.521 1.00 23.54
ATOM	1882 CB GLU 403	-4.274 9.482 28.562 1.00 63.22
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ATOM	1.883	CG GLU	403	-5.469 8.531 28.506 1.00 63.22
ATOM	1884	CD GLU	403	-6.530 8.952 27.498 1.00 63.22
ATOM	1885	OE1 GLU	403	
ATOM	1886	OE2 GLU	403	
ATOM	1887	C GLU	403	-2.708 7.629 29.170 1.00 23.54
ATOM	1888	O- GLU	403	-3.210 6.656 29.735 1.00 63.22
ATOM	1889	N VAL	404	-1.787 7.515 28.221 1.00 33.24
ATOM	1890	CA VAL	404	-1.297 6.213 27.782 1.00 33.24
ATOM	1891	CB VAL	404	-0.621 6.314 26.390 1.00 30.71
ATOM	1892	CG1 VAL	404	
ATOM	1893	CG2 VAL	404	
ATOM	1894	C VAL	404	-0.338 5.528 28.752 1.00 33.24
ATOM	1895	O VAL	404	-0.386 4.305 28.914 1.00 30.71
ATOM		N PHE	405	0.526 6.309 29.392 1.00 33.66
ATOM		CA PHE	405	1.516 5.752 30.308 1.00 33.66
ATOM		CB PHE	405	2.901 6.326 29.984 1.00 34.35
ATOM		CG PHE	405	
ATOM		CD1 PHE	405	3.519 7.134 27.683 1.00 34.35
ATOM		CD2 PHE	405	3.569 4.782 28.114 1.00 34.35
ATOM		CE1 PHE	405	3.911 6.906 26.365 1.00 34.35
ATOM		CE2 PHE	405	3.960 4.545 26.798 1.00 34.35
ATOM		CZ PHE	405	4.131 5.610 25.922 1.00 34.35
ATOM		C PHE	405	1.189 5.931 31.790 1.00 33.66
ATOM		O PHE	405	2.036 5.539 32.623 1.00 34.35
ATOM		OXT PHE	405	0.090 6.434 32.107 1.00 34.35
ATOM		C1 TRI	1	8.375 7.063 18.475 1.00 34.21
ATOM		C2 TRI	1	10.048 8.688 23.016 1.00 33.36
ATOM	1910	C3 TRI	1	8.104 8.391 18.941 1.00 34.21
ATOM	1911	C4 TRI	1	10.496 9.696 23.813 1.00 33.36
ATOM	1912	C5 TRI	1	8.916 8.943 19.927 1.00 34.21
ATOM	1913 C	C6 TRI	1	10.152 9.772 25.121 1.00 33.36
ATOM	1914 C	7 TRI	1	9.862 8.178 20.609 1.00 34.21
ATOM	1915 C	C8 TRI	1	9.246 8.821 25.653 1.00 33.36
ATOM	1916 C	9 TRI	1	10.117 6.865 20.147 1.00 34.21
ATOM	1917 C	C10 TRI	1	8.805 7.754 24.847 1.00 33.36
ATOM	1918 C	C11 TRI	1	9.375 6.339 19.026 1.00 34.21
ATOM	1919 C	C12 TRI	1	9.125 7.756 23.490 1.00 33.36
ATOM	1920 C	13 TRI	1	7.540 6.470 17.383 1.00 35.85
ATOM	1921 C	15 TRI	1	8.158 6.555 15.938 1.00 35.85
ATOM	1922 I	l TRI	1	8.713 10.990 20.395 1.00 34.21
ATOM	1923 I	2 TRI		10.951 11.289 26.315 1.00 33.36
ATOM				11.592 5.685 21.118 1.00 34.21
ATOM	1925 O		1	9.407 6.654 15.852 1.00 35.85
ATOM		2 TRI	1	10.570 8.649 21.717 1.00 33.36
ATOM	1927 O		1	8.798 8.969 26.979 1.00 33.36
ATOM		4 TRI	1	7.352 6.522 14.973 1.00 35.85
ATOM	1929 O		501	9.189 2.098 11.091 1.00 33.36
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ATOM	1930	01	HOH	503	5.152 5.261 12.137 1.00 33.36
ATOM	1931	01	HOH	504	3.970 5.057 16.390 1.00 33.36
ATOM	1932	01	HOH	534	8.296 -0.941 8.998 1.00 33.36
ATOM	1933	01	HOH	538	4.845 14.369 13.635 1.00 33.36
ATOM	1934	01	HOH	540	5.789 12.049 10.352 1.00 33.36
ATOM	1936	01	HOH	555	5.721 2.525 28.939 1.00 33.36
ATOM	1937	01	HOH	556	3.732 1.273 26.724 1.00 33.36
ATOM	1935	01	HOH	600	8.767 4.847 8.517 1.00 33.36
ATOM	1938	AS	l CAD	701	1.863 1.579 0.837 1.00 37.00
ATOM	1939	C2	CAD	701	1.760 -0.100 0.335 1.00 33.36
ATOM	1940	C3	CAD	701	3.511 1.872 1.858 1.00 28.02
ATOM	1941	04	CAD	701	1.785 2.506 -0.433 1.00 28.02
ATOM	1942	O5	CAD	701	0.592 2.019 1.654 1.00 28.02
ATOM	1943	AS	AS	801	11.254 16.718 33.126 1.00 37.00 AS
ATOM	1944	AS	AS	802	16.338 -1.161 29.914 1.00 37.00 AS
ATOM	1945	AS	AS	803	-14.931 -11.763 25.324 1.00 37.00 AS
END					

APPENDIX 5

TR IPBR2.PDB

REMARK rTR ipbr2 full length numbering REMARK . REMARK Rfactor 0.214 Rfree 0.224 REMARK Resolution 15. 2.2 all reflections REMARK REMARK Three cacodylate-modified cysteines (CYA) REMARK Cya334, Cya380, Cya392 REMARK cacodylate modeled as single arsenic atom REMARK REMARK side chain of certain residues modeled as ALA due to poor density: REMARK however, residue name reflects true residue for clarity REMARK REMARK clone obtained from Murray et. al. REMARK deposited sequence confirmed, REMARK differing from that reported by Thompson et. al. REMARK in the following codons: REMARK 281 Thr - Ala REMARK 285 Lys - Glu REMARK identical to that reported by Mitsuhashi et. al. REMARK gb:RNTRAVI X07409 JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY, M.J.MACDONALD JRNL **AUTH 2 H.C.TOWLE** TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES JRNL FOR TWO **JRNL** TITL 2 DISTINCT THYROID HORMONE RECPTORS JRNL REF **JBC** V. 263 25 1988 JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS JRNL TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR **EXPRESSED** JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM JRNL **SCIENCE** V. 237 1987 JRNL AUTH T.MITSUHASHI, G. TENNYSON, V. NIKODEM JRNL TITL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY **ALTERNATIVE** TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE JRNL TRANSCRIPT JRNL REF NUC. ACIDS. RES. V. 16 12 1988 REMARK ATOM 1 CB ARG 157 68.481 10.663 6.906 1.00 57.50

69.793 10.213 7.512 1.00 59.93

70.510 11.365 8.189 1.00 70.24

21388546 232

2 CG ARG 157

3 CD ARG 157

ATOM

ATOM

ATOM	4 NE ARG 157	71.661 10.906 8.961 1.00 77.62
ATOM	5 CZ ARG 157	71.599 10.492 10.224 1.00 78.75
ATOM	6 NH1 ARG 157	70.440 10.480 10.870 1.00 74.33
ATOM	7 NH2 ARG 157	72.697 10.075 10.839 1.00 83.44
ATOM	8 C ARG 157	66.314 10.014 5.809 1.00 46.84
ATOM	9 O ARG 157	66.109 10.397 4.659 1.00 54.49
ATOM	10 N ARG 157	68.442 9.069 5.013 1.00 56.54
ATOM	11 CA ARG 157	67.704 9.537 6.222 1.00 52.92
ATOM	12 N PRO 158	65.335 9.953 6.727 1.00 39.44
ATOM	13 CD PRO 158	65.503 9.448 8.099 1.00 41.72
ATOM	14 CA PRO 158	63.946 10.368 6.487 1.00 34.98
ATOM	15 CB PRO 158	63.282 10.172 7.854 1.00 34.92
ATOM	16 CG PRO 158	64.096 9.096 8.487 1.00 45.83
ATOM	17 C PRO 158	63.765 11.804 5.992 1.00 34.13
ATOM	18 O PRO 158	64.223 12.757 6.621 1.00 31.07
ATOM	19 N GLU 159	63.110 11.932 4.841 1.00 31.36
ATOM	20 CA GLU 159	62.814 13.220 4.228 1.00 27.34
ATOM	21 CB GLU 159	62.569 13.041 2.726 1.00 24.27
ATOM	22 CG GLU 159	63.814 12.866 1.887 1.00 24.85
ATOM	23 CD GLU 159	64.409 14.188 1.454 1.00 28.12
ATOM	24 OE1 GLU 159	63.642 15.144 1.224 1.00 29.26
ATOM	25 OE2 GLU 159	65.646 14.269 1.326 1.00 29.52
ATOM	26 C GLU 159	61.528 13.707 4.870 1.00 24.30
ATOM	27 O GLU 159	60.855 12.934 5.566 1.00 29.01
ATOM	28 N PRO 160	61.192 14.989 4.718 1.00 24.62
ATOM	29 CD PRO 160	61.979 16.126 4.188 1.00 18.72
ATOM	30 CA PRO 160	59.947 15.451 5.330 1.00 21.62
ATOM	31 CB PRO 160	59.945 16.955 5.048 1.00 12.71
ATOM	32 CG PRO 160	61.394 17.297 4.930 1.00 15.12
ATOM	33 C PRO 160	58.743 14.752 4.671 1.00 24.61
ATOM	34 O PRO 160	58.789 14.384 3.490 1.00 22.63
ATOM	35 N THR 161	57.705 14.504 5.450 1.00 25.86
ATOM	36 CA THR 161	56.515 13.864 4.921 1.00 23.77
ATOM	37 CB THR 161	55.689 13.201 6.048 1.00 21.75
ATOM	38 OG1 THR 161	55.178 14.210 6.926 1.00 20.78
ATOM	39 CG2 THR 161	56.549 12.227 6.847 1.00 18.44
ATOM	40 C THR 161	55.680 14.967 4.269 1.00 28.67
ATOM	41 O THR 161	55.917 16.151 4.510 1.00 29.90
ATOM	42 N PRO 162	54.685 14.597 3.448 1.00 27.79
ATOM	43 CD PRO 162	54.313 13.237 3.019 1.00 23.25
ATOM	44 CA PRO 162	53.843 15.603 2.795 1.00 26.19
ATOM	45 CB PRO 162	52.699 14.766 2.227 1.00 19.89
ATOM	46 CG PRO 162	53.394 13.492 1.848 1.00 20.63
ATOM	47 C PRO 162	53.334 16.661 3.775 1.00 24.81
ATOM	48 O PRO 162	53.477 17.863 3.526 1.00 21.10
ATOM	49 N GLU 163	52.812 16.198 4.911 1.00 26.34
ATOM	50 CA GLU 163	52.266 17.065 5.959 1.00 30.38

ATOM	51 CB GLU 163	51.640 16.231 7.086 1.00 29.46
ATOM	52 CG GLU 163	50.482 15.321 6.666 1.00 48.37
ATOM	53 CD GLU 163	50.918 14.132 5.816 1.00 53.12
ATOM	54 OE1 GLU 163	51.890 13.441 6.194 1.00 52.22
ATOM	55 OE2 GLU 163	50.282 13.886 4.766 1.00 59.14
ATOM	56 C GLU 163	53.353 17.949 6.552 1.00 26.74
ATOM	57 O GLU 163	
ATOM	58 N GLU 164	
ATOM		54.553 17.389 6.677 1.00 26.74
		55.679 18.124 7.221 1.00 23.65
ATOM	60 CB GLU 164	56.805 17.174 7.609 1.00 18.85
ATOM	61 CG GLU 164	56.441 16.306 8.804 1.00 26.81
ATOM	62 CD GLU 164	57.536 15.334 9.188 1.00 31.06
ATOM	63 OE1 GLU 164	58.404 15.050 8.340 1.00 29.21
ATOM	64 OE2 GLU 164	57.524 14.848 10.340 1.00 31.39
ATOM	65 C GLU 164	56.165 19.204 6.276 1.00 26.54
ATOM	66 O GLU 164	56.609 20.258 6.724 1.00 32.48
ATOM	67 N TRP 165	56.075 18.957 4.971 1.00 23.41
ATOM	68 CA TRP 165	56.488 19.962 3.998 1.00 20.81
ATOM	69 CB TRP 165	56.462 19.405 2.573 1.00 18.15
ATOM	70 CG TRP 165	57.762 18.747 2.164 1.00 15.80
ATOM	71 CD2 TRP 165	59.058 19.377 2.064 1.00 15.35
ATOM	72 CE2 TRP 165	59.959 18.392 1.628 1.00 12.14
ATOM	73 CE3 TRP 165	59.527 20.676 2.287 1.00 17.56
ATOM	74 CD1 TRP 165	57.939 17.449 1.804 1.00 12.78
ATOM	75 NE1 TRP 165	59.253 17.230 1.484 1.00 16.10
ATOM	76 CZ2 TRP 165	61.318 18.657 1.419 1.00 16.26
ATOM	77 CZ3 TRP 165	60.879 20.944 2.079 1.00 19.52
ATOM	78 CH2 TRP 165	61.760 19.933 1.642 1.00 16.48
ATOM	79 C TRP 165	55.547 21.151 4.109 1.00 19.66
ATOM	80 O TRP 165	55.975 22.295 3.960 1.00 23.61
ATOM	81 N ASP 166	54.269 20.882 4.376 1.00 22.66
ATOM	82 CA ASP 166	53.269 21.943 4.537 1.00 22.00
ATOM	83 CB ASP 166	
ATOM	84 CG ASP 166	
		51.347 20.681 3.458 1.00 31.41
ATOM	85 OD1 ASP 166	51.816 21.028 2.360 1.00 26.38
ATOM	86 OD2 ASP 166	50.464 19.803 3.570 1.00 32.25
ATOM	87 C ASP 166	53.631 22.760 5.773 1.00 26.47
ATOM	88 O ASP 166	53.694 23.991 5.718 1.00 30.25
ATOM	89 N LEU 167	53.887 22.054 6.872 1.00 24.12
ATOM	90 CA LEU 167	54.268 22.663 8.139 1.00 26.44
ATOM	91 CB LEU 167	54.596 21.557 9.148 1.00 32.57
ATOM	92 CG LEU 167	54.659 21.919 10.629 1.00 36.97
ATOM	93 CD1 LEU 167	53.289 22.402 11.080 1.00 43.83
ATOM	94 CD2 LEU 167	55.096 20.712 11.448 1.00 34.75
ATOM	95 C LEU 167	55.501 23.533 7.904 1.00 23.19
ATOM	96 O LEU 167	55.570 24.670 8.368 1.00 28.18
ATOM	97 N ILE 168	56.450 22.988 7.147 1.00 19.25

ATOM	98 CA ILE 168	57.703 23.651 6.801 1.00 17.71
ATOM	99 CB ILE 168	58.632 22.693 6.006 1.00 14.43
ATOM	100 CG2 ILE 168	59.740 23.451 5.304 1.00 16.71
ATOM	101 CG1 ILE 168	59.219 21.644 6.948 1.00 21.24
ATOM	102 CD1 ILE 168	60.063 20.588 6.264 1.00 18.18
ATOM	103 C- ILE 168	57.475 24.931 6.002 1.00 28.73
ATOM	104 O ILE 168	58.064 25.977 6.307 1.00 29.36
ATOM	105 N HIS 169	56.601 24.866 5.005 1.00 24.43
ATOM	106 CA HIS 169	56.319 26.027 4.169 1.00 23.64
ATOM	107 CB HIS 169	55.459 25.631 2.971 1.00 23.55
ATOM	108 CG HIS 169	56.140 24.683 2.034 1.00 23.82
ATOM	109 CD2 HIS 169	57.455 24.429 1.824 1.00 19.23
ATOM	110 ND1 HIS 169	55.450 23.833 1.199 1.00 22.92
ATOM	111 CE1 HIS 169	56.302 23.089 0.522 1.00 19.56
ATOM	112 NE2 HIS 169	57.527 23.431 0.883 1.00 26.00
ATOM	113 C HIS 169	55.653 27.135 4.962 1.00 19.37
ATOM	114 O HIS 169	56.069 28.288 4.880 1.00 25.64
ATOM	115 N VAL 170	54.638 26.782 5.745 1.00 19.88
ATOM	116 CA VAL 170	53.925 27.758 6.555 1.00 20.28
ATOM	117 CB VAL 170	52.755 27.100 7.330 1.00 26.06
ATOM	118 CG1 VAL 170	52.093 28.109 8.259 1.00 20.15
ATOM	119 CG2 VAL 170	51.725 26.541 6.352 1.00 18.69
ATOM	120 C VAL 170	54.886 28.442 7.532 1.00 23.11
ATOM	121 O VAL 170	54.907 29.672 7.625 1.00 28.86
ATOM	122 N ALA 171	55.716 27.644 8.203 1.00 20.48
ATOM	123 CA ALA 171	56.686 28.146 9.173 1.00 19.84
ATOM	124 CB ALA 171	57.365 26.985 9.902 1.00 18.07
ATOM	125 C ALA 171	57.728 29.049 8.512 1.00 20.62
ATOM	126 O ALA 171	58.033 30.127 9.037 1.00 24.67
ATOM	127 N THR 172	58.251 28.632 7.359 1.00 20.65
ATOM	128 CA THR 172	59.247 29.428 6.640 1.00 18.91
ATOM	129 CB THR 172	59.755 28.709 5.380 1.00 20.06
ATOM	130 OG1 THR 172	60.267 27.417 5.734 1.00 20.30
ATOM	131 CG2 THR 172	60.877 29.516 4.726 1.00 18.38
ATOM	132 C THR 172	58.675 30.786 6.235 1.00 24.43
ATOM	133 O THR 172 134 N GLU 173	59.346 31.815 6.360 1.00 23.54 57.430 30.702 5.766 1.00 24.33
ATOM ATOM		57.430 30.792 5.766 1.00 24.33 56.783 32.031 5.361 1.00 25.08
ATOM		56.783 32.031 5.361 1.00 25.98 55.460 31.734 4.651 1.00 28.39
ATOM	136 CB GLU 173 137 CG GLU 173	
ATOM	137 CG GLU 173 138 CD GLU 173	54.679 32.974 4.207 1.00 40.39 55.487 33.951 3.347 1.00 48.33
ATOM		
ATOM		55.261 35.172 3.478 1.00 51.86
ATOM	140 OE2 GLU 173 141 C GLU 173	56.334 33.513 2.533 1.00 46.92 56.564 32.953 6.562 1.00 25.57
ATOM	141 C GLU 173	
ATOM	142 O GLU 173 143 N ALA 174	56.877 34.141 6.498 1.00 27.76 56.071 32.383 7.664 1.00 25.31
ATOM	144 CA ALA 174	55.823 33.128 8.900 1.00 22.66
711 0141	· ·	33.023 33.120 6.900 1.00 22.00

ATOM	145 CB ALA 174	55.340 32.183 10.000 1.00 18.21
ATOM	146 C ALA 174	57.097 33.847 9.338 1.00 23.47
ATOM	147 O ALA 174	57.056 35.003 9.755 1.00 23.76
ATOM	148 N HIS 175	58.233 33.168 9.226 1.00 22.22
ATOM	149 CA HIS 175	59.503 33.769 9.592 1.00 20.21
ATOM	150 CB HIS 175	60.586 32.700 9.738 1.00 13.82
ATOM	151 CG HIS 175	61.950 33.261 9.984 1.00 20.53
ATOM	152 CD2 HIS 175	62.378 34.221 10.843 1.00 10.04
ATOM	153 ND1 HIS 175	63.054 32.890 9.249 1.00 22.39
ATOM	154 CE1 HIS 175	64.103 33.596 9.640 1.00 13.46
ATOM	155 NE2 HIS 175	63.715 34.410 10.605 1.00 20.86
ATOM	156 C HIS 175	59.949 34.822 8.571 1.00 25.39
ATOM	157 O HIS 175	60.370 35.920 8.949 1.00 26.31
ATOM	158 N ARG 176	59.868 34.494 7.284 1.00 23.17
ATOM	159 CA ARG 176	60.292 35.423 6.239 1.00 24.26
ATOM	160 CB ARG 176	60.168 34.767 4.872 1.00 30.31
ATOM	161 CG ARG 176	61.286 33.793 4.576 1.00 39.36
ATOM	162 CD ARG 176	61.049 33.139 3.243 1.00 49.23
ATOM	163 NE ARG 176	62.188 32.346 2.808 1.00 60.62
ATOM	164 CZ ARG 176	62.230 31.688 1.653 1.00 67.96
ATOM	165 NH1 ARG 176	61.192 31.731 0.823 1.00 68.84
ATOM	166 NH2 ARG 176	63.313 30.999 1.321 1.00 67.97
ATOM	167 C ARG 176	59.548 36.749 6.267 1.00 23.09
ATOM	168 O ARG 176	60.163 37.807 6.173 1.00 30.71
ATOM	169 N SER 177	58.240 36.686 6.488 1.00 22.69
ATOM	170 CA SER 177	57.416 37.885 6.536 1.00 26.50
ATOM	171 CB SER 177	55.946 37.520 6.341 1.00 19.42
ATOM	172 OG SER 177	55.507 36.611 7.331 1.00 27.68
ATOM	173 C SER 177	57.574 38.695 7.821 1.00 28.70
ATOM	174 O SER 177	56.986 39.772 7.948 1.00 34.31
ATOM	175 N THR 178	58.327 38.165 8.786 1.00 27.42
ATOM	176 CA THR 178	58.540 38.850 10.060 1.00 21.88
ATOM	177 CB THR 178	
ATOM	178 OG1 THR 178	58.354 36.776 11.337 1.00 24.26
ATOM	179 CG2 THR 178	56.344 38.037 10.994 1.00 16.77
ATOM	180 C THR 178	60.027 39.018 10.375 1.00 23.86
ATOM	181 O THR 178	60.399 39.439 11.474 1.00 24.64
ATOM	182 N ASN 179	60.873 38.690 9.402 1.00 23.79
ATOM	183 CA ASN 179	62.315 38.813 9.563 1.00 26.01
ATOM	184 CB ASN 179	63.018 37.607 8.947 1.00 23.77
ATOM	185 CG ASN 179	64.451 37.495 9.386 1.00 30.79
ATOM	186 OD1 ASN 179	64.737 37.376 10.575 1.00 36.19
ATOM	187 ND2 ASN 179	65.364 37.516 8.432 1.00 35.34
ATOM	188 C ASN 179	62.767 40.101 8.875 1.00 32.11
ATOM	189 O ASN 179	62.947 40.136 7.652 1.00 36.36
ATOM	190 N ALA 180	
ATOM	191 CA ALA 180	63.333 42.473 9.179 1.00 28.75

ATOM	192 CB ALA 180	63.653 43.390 10.346 1.00 29.96
ATOM	193 C ALA 180	64.481 42.481 8.182 1.00 37.02
ATOM	194 O ALA 180	65.518 41.866 8.414 1.00 41.85
ATOM	195 N GLN 181	64.266 43.163 7.057 1.00 37.15
ATOM	196 CA GLN 181	65.261 43.306 5.995 1.00 39.33
ATOM	197 CB GLN 181	66.572 43.877 6.552 1.00 37.42
ATOM	198 CG GLN 181	66.420 45.190 7.309 1.00 44.86
ATOM	199 CD GLN 181	65.779 46.285 6.479 1.00 53.60
ATOM	200 OE1 GLN 181	64.712 46.793 6.821 1.00 58.51
ATOM	201 NE2 GLN 181	66.422 46.650 5.378 1.00 63.36
ATOM	202 C GLN 181	65.549 42.053 5.164 1.00 44.18
ATOM	203 O GLN 181	66.367 42.102 4.239 1.00 46.35
ATOM	204 N GLY 182	64.873 40.949 5.474 1.00 43.76
ATOM	205 CA GLY 182	65.074 39.713 4.732 1.00 46.26
ATOM	206 C GLY 182	66.531 39.363 4.477 1.00 49.98
ATOM	207 O. GLY 182	67.309 39.175 5.419 1.00 56.26
ATOM	208 N SER 183	66.907 39.274 3.205 1.00 50.96
ATOM	209 CA SER 183	68.281 38.947 2.830 1.00 55.69
ATOM	210 CB SER 183	68.284 38.024 1.608 1.00 56.52
ATOM	211 OG SER 183	67.398 38.497 0.609 1.00 60.82
ATOM	212 C SER 183	69.121 40.197 2.558 1.00 59.84
ATOM	213 O SER 183	70.352 40.138 2.540 1.00 66.02
ATOM	214 N HIS 184	68.453 41.338 2.413 1.00 60.68
ATOM	215 CA HIS 184	69.131 42.600 2.139 1.00 60.01
ATOM	216 CB HIS 184	68.150 43.596 1.517 1.00 53.49
ATOM	217 C HIS 184	69.798 43.209 3.380 1.00 59.43
ATOM	218 O HIS 184	70.373 44.300 3.303 1.00 59.56
ATOM	219 N TRP 185	69.753 42.500 4.508 1.00 57.54
ATOM	220 CA TRP 185	70.343 42.995 5.754 1.00 54.25
ATOM	221 CB TRP 185	70.147 41.988 6.899 1.00 47.54
ATOM	222 CG TRP 185	70.905 40.692 6.752 1.00 41.08
ATOM	223 CD2 TRP 185	72.233 40.404 7.230 1.00 39.59
ATOM	224 CE2 TRP 185	72.522 39.070 6.874 1.00 30.27
ATOM	225 CE3 TRP 185	73.202 41.146 7.919 1.00 35.23
ATOM	226 CD1 TRP 185	70.462 39.553 6.149 1.00 39.73
ATOM	227 NE1 TRP 185	71.427 38.577 6.219 1.00 40.01
ATOM	228 CZ2 TRP 185	73.740 38.457 7.188 1.00 31.35
ATOM	229 CZ3 TRP 185	74.416 40.535 8.230 1.00 32.76
ATOM	230 CH2 TRP 185	74.673 39.203 7.861 1.00 31.71
ATOM	231 C TRP 185	71.818 43.382 5.655 1.00 54.21
ATOM	232 O TRP 185	72.229 44.403 6.200 1.00 52.82
ATOM	233 N LYS 186	72.605 42.584 4.938 1.00 54.57
ATOM	234 CA LYS 186	74.034 42.848 4.788 1.00 55.46
ATOM	235 CB LYS 186	74.712 41.682 4.080 1.00 53.31
ATOM	236 C LYS 186	74.338 44.160 4.061 1.00 58.96
ATOM	237 O LYS 186	75.417 44.731 4.226 1.00 62.57
ATOM	238 N GLN 187	73.382 44.640 3.268 1.00 60.12

239 CA GLN **ATOM** 187 73.563 45.873 2.512 1.00 60.15 **ATOM** 240 CB GLN 187 73.157 45.653 1.050 1.00 57.00 **ATOM** 241 C GLN 187 72.809 47.064 3.101 1.00 60.91 **ATOM** 242 O **GLN** 187 73.149 48.213 2.822 1.00 66.50 **ATOM** 243 N **ARG** 188 71.795 46.790 3.919 1.00 59.55 **ATOM** 244 CA ARG 70.983 47.847 188 4.525 1.00 59.26 **ATOM** 245 CB ARG 188 69.504 47.462 4.466 1.00 55.21 ATOM 246 C ARG 188 71.372 48.243 5.959 1.00 58.97 **ATOM** 247 O **ARG** 188 70.914 49.269 6.469 1.00 58.54 248 N **ATOM ARG** 189 72.202 47.432 6.607 1.00 55.46 **ATOM** 249 CA ARG 189 72.630 47.704 7.979 1.00 52.98 **ATOM** 250 CB ARG 189 73.211 46.437 8.619 1.00 47.73 **ATOM** 251 CG ARG 189 74.509 45.985 7.989 1.00 47.88 **ATOM** 252 CD ARG 189 75.080 44.763 8.654 1.00 46.96 **ATOM** 253 NE ARG 189 76.377 44.441 8.068 1.00 57.93 **ATOM** 254 CZ ARG 189 77.450 44.090 8.768 1.00 64.81 **ATOM** 255 NH1 ARG 77.385 44.005 10.087 1.00 67.27 189 **ATOM** 256 NH2 ARG 189 78.600 43.860 8.148 1.00 67.84 **ATOM** 257 C ARG 189 73.650 48.838 8.091 1.00 53.48 **ATOM** 258 O ARG 189 74.513 49.004 7.227 1.00 57.14 **ATOM** 259 N LYS 190 73.533 49.617 9.161 1.00 51.31 **ATOM** 260 CA LYS 190 74.444 50.722 9.435 1.00 48.83 **ATOM** 261 CB LYS 190 73.682 52.036 9.516 1.00 45.36 262 C LYS ATOM 190 75.101 50.411 10.773 1.00 46.88 **ATOM** 263 O LYS 190 74.454 49.872 11.675 1.00 48.81 **ATOM** 264 N PHE 191 76.385 50.724 10.894 1.00 46.98 **ATOM 265 CA PHE** 191 77.123 50.462 12.125 1.00 44.38 **ATOM 266 CB PHE** 78.630 50.520 11.873 1.00 44.25 191 **ATOM 267 CG PHE** 191 79.170 49.336 11.123 1.00 49.51 **ATOM** 268 CD1 PHE 191 78.828 49.124 9.791 1.00 52.20 **ATOM** 269 CD2 PHE 191 80.029 48.437 11.748 1.00 47.25 **ATOM** 270 CE1 PHE 191 79.335 48.031 9.090 1.00 55.86 **ATOM** 271 CE2 PHE 191 80.542 47.343 11.059 1.00 49.73 272 CZ PHE **ATOM** 191 80.195 47.139 9.727 1.00 51.55 **ATOM** PHE 273 C 191 76.764 51.443 13.233 1.00 46.44 **ATOM** 274 O PHE 191 76.647 52.645 12.996 1.00 51.28 **ATOM** 275 N LEU 192 76.567 50.924 14.439 1.00 47.66 **ATOM 276 CA LEU** 192 76.256 51.776 15.577 1.00 46.44 **ATOM 277 CB LEU** 192 75.930 50.924 16.808 1.00 38.06 **ATOM** 278 CG LEU 192 75.527 51.672 18.082 1.00 33.55 **ATOM** 279 CD1 LEU 192 74.180 52.339 17.871 1.00 28.17 **ATOM** 280 CD2 LEU 192 75.476 50.717 19.268 1.00 26.95 **ATOM** 192 281 C LEU 77.524 52.595 15.824 1.00 45.82 **ATOM** 282 O LEU 192 78.604 52.024 16.008 1.00 41.65 **ATOM** 283 N PRO 193 77.422 53.936 15.782 1.00 48.88 **ATOM** 284 CD PRO 193 76.176 54.701 15.577 1.00 47.51 **ATOM** 285 CA PRO 193 78.560 54.836 15.999 1.00 47.34

ATOM 286 CB PRO 193 77.879 56.162 16.319 1.00 46.04 **ATOM** 287 CG PRO 193 76.675 56.126 15.438 1.00 46.24 **ATOM** 288 C **PRO** 193 79.475 54.377 17.137 1.00 49.60 289 O **ATOM PRO** 193 79.000 54.033 18.218 1.00 54.05 **ATOM** 290 N **ASP** 194 80.783 54.383 16.891 1.00 50.63 **ATOM** 291 CA ASP 194 81.769 53.951 17.885 1.00 54.57 292 CB ASP **ATOM** 194 83.164 53.965 17.272 1.00 59.28 **ATOM** 293 CG ASP 194 83.309 52.952 16.170 1.00 66.39 **ATOM** 294 OD1 ASP 194 83.057 53.311 14.998 1.00 72.95 **ATOM** 295 OD2 ASP 194 83.640 51.787 16.486 1.00 69.00 **ATOM** 296 C **ASP** 194 81.769 54.726 19.198 1.00 54.41 **ATOM** 297 O **ASP** 194 82.229 54.221 20.222 1.00 55.27 **ATOM** 298 N **ASP** 195 81.268 55.956 19.168 1.00 57.20 **ATOM** 299 CA ASP 195 81.206 56.775 20.371 1.00 59.68 **ATOM** 300 CB ASP 195 81.017 58.261 20.006 1.00 62.99 **ATOM 301 CG ASP** 195 79.747 58.526 19.187 1.00 71.67 **ATOM 302 OD1 ASP** 195 78.734 58.956 19.796 1.00 70.17 **ATOM** 303 OD2 ASP 195 79.782 58.311 17.951 1.00 75.23 **ATOM** 304 C ASP 195 80.092 56.289 21.306 1.00 58.39 **ATOM ASP** 305 O 195 80.032 56.676 22.474 1.00 59.81 **ATOM** 306 N ILE 196 79.245 55.399 20.794 1.00 54.47 **ATOM 307 CA ILE** 196 78.141 54.840 21.568 1.00 49.00 **ATOM** 308 CB ILE 196 76.839 54.780 20.731 1.00 46.64 **ATOM** 309 CG2 ILE 196 75.701 54.195 21.560 1.00 42.11 **ATOM** 310 CG1 ILE 196 76.467 56.184 20.241 1.00 44.23 **ATOM** 311 CD1 ILE 196 75.214 56.238 19.373 1.00 48.45 **ATOM** 312 C ILE 196 78.497 53.436 22.068 1.00 46.22 ILE **ATOM** 313 O 196 78.912 52.570 21.298 1.00 42.07 **ATOM** 314 N GLY 197 78.357 53.228 23.370 1.00 45.62 **ATOM** 315 CA GLY 197 78.658 51.930 23.941 1.00 51.49 **ATOM** 316 C **GLY** 197 80.005 51.832 24.625 1.00 54.64 **ATOM** 317 O **GLY** 197 80.377 50.759 25.092 1.00 49.98 **ATOM** 318 N GLN 198 80.726 52.946 24.725 1.00 60.08 **ATOM** 319 CA GLN 198 82.039 52.939 25.366 1.00 61.01 **ATOM** 320 CB GLN 198 83.082 53.568 24.441 1.00 55.55 **ATOM** 321 C GLN 198 82.044 53.633 26.733 1.00 59.57 **ATOM** 322 O **GLN** 198 83.103 54.016 27.232 1.00 61.30 **ATOM** 323 N SER 199 80.875 53.738 27.362 1.00 57.27 **ATOM** 324 CA SER 199 80.758 54.397 28.665 1.00 50.61 **ATOM** 325 CB SER 199 80.276 55.842 28.478 1.00 53.70 **ATOM** 326 OG SER 199 81.010 56.508 27.463 1.00 61.92 **ATOM** 327 C SER 199 79.848 53.684 29.675 1.00 46.41 **ATOM** 328 O **SER** 199 78.798 54.210 30.060 1.00 41.16 **ATOM** 200 329 N PRO 80.222 52.466 30.096 1.00 42.08 **ATOM** 81.349 51.648 29.605 1.00 38.31 330 CD PRO 200 **ATOM** 200 79.409 51.722 31.065 1.00 44.04 331 CA PRO **ATOM** 332 CB PRO 200 79.941 50.297 30.925 1.00 36.06

ATOM		81.377 50.504 30.583 1.00 37.43
ATOM	334 C PRO 200	79.615 52.270 32.485 1.00 50.91
ATOM	335 O PRO 200	80.629 51.980 33.123 1.00 55.65
ATOM	336 N ILE 201	78.663 53.060 32.975 1.00 55.81
ATOM	337 CA ILE 201	78.781 53.651 34.311 1.00 57.24
ATOM	338 CB ILE 201	78.861 55.192 34.250 1.00 58.40
ATOM	339 CG2 ILE 201	80.218 55.622 33.709 1.00 60.49
ATOM	340 CG1 ILE 201	77.716 55.751 33.404 1.00 62.42
ATOM	341 CD1 ILE 201	77.819 57.234 33.137 1.00 61.68
ATOM	342 C ILE 201	77.728 53.241 35.332 1.00 56.52
ATOM	343 O ILE 201	77.961 53.352 36.537 1.00 60.89
ATOM	344 N VAL 202	76.564 52.794 34.871 1.00 52.76
ATOM	345 CA VAL 202	75.522 52.366 35.802 1.00 47.37
ATOM	346 CB VAL 202	74.117 52.377 35.153 1.00 38.14
ATOM	347 CG1 VAL 202	73.092 51.804 36.117 1.00 30.35
ATOM	348 CG2 VAL 202	73.730 53.798 34.763 1.00 26.69
ATOM	349 C VAL 202	75.885 50.958 36.285 1.00 53.65
ATOM	350 O VAL 202	75.914 50.010 35.500 1.00 55.10
ATOM	351 N SER 203	76.226 50.839 37.561 1.00 59.85
ATOM	352 CA SER 203	76.614 49.556 38.132 1.00 64.58
ATOM	353 CB SER 203	77.209 49.749 39.532 1.00 68.95
ATOM	354 OG SER 203	78.396 50.523 39.483 1.00 74.02
ATOM	355 C SER 203	75.493 48.528 38.197 1.00 61.69
ATOM	356 O SER 203	74.351 48.846 38.535 1.00 63.63
ATOM	357 N MET 204	75.848 47.295 37.859 1.00 57.37
ATOM	358 CA MET 204	74.932 46.162 37.885 1.00 57.54
ATOM	359 CB MET 204	74.847 45.505 36.501 1.00 56.59
ATOM	360 CG MET 204	74.012 46.270 35.489 1.00 44.08
ATOM	361 SD MET 204	72.255 46.228 35.884 1.00 46.62
ATOM	362 CE MET 204	71.775 44.758 35.013 1.00 48.37
ATOM	363 C MET 204	75.522 45.178 38.888 1.00 55.86
ATOM	364 O MET 204	76.746 45.089 39.027 1.00 58.94
ATOM	365 N PRO 205	74.671 44.432 39.607 1.00 55.36
ATOM	366 CD PRO 205	73.203 44.570 39.625 1.00 57.73
ATOM	367 CA PRO 205	75.119 43.453 40.604 1.00 56.82
ATOM	368 CB PRO 205	73.814 43.042 41.295 1.00 59.79
ATOM	369 CG PRO 205	72.769 43.281 40.255 1.00 57.85
ATOM	370 C PRO 205	75.902 42.239 40.083 1.00 57.25
ATOM	371 O PRO 205	75.683 41.118 40.541 1.00 66.28
ATOM	372 N ASP 206	76.822 42.462 39.147 1.00 58.75
ATOM	373 CA ASP 206	77.639 41.389 38.586 1.00 61.09
ATOM	374 CB ASP 206	76.802 40.462 37.685 1.00 66.07
ATOM	375 CG ASP 206	76.158 41.190 36.521 1.00 70.97
ATOM	376 OD1 ASP 206	74.989 41.613 36.662 1.00 76.97
ATOM	377 OD2 ASP 206	76.813 41.322 35.465 1.00 61.12
ATOM	378 C ASP 206	78.865 41.910 37.832 1.00 61.96
ATOM	379 O ASP 206	79.406 41.230 36.957 1.00 65.14

ATOM 380 N GLY 207 79.282 43.130 38.158 1.00 63.00 **ATOM** 381 CA GLY 207 80.455 43.709 37.522 1.00 64.43 **ATOM** 382 C GLY 207 80.224 44.467 36.229 1.00 64.81 **ATOM** 383 O **GLY** 207 80.649 45.619 36.110 1.00 68.76 **ATOM** 384 N **ASP** 208 79.584 43.827 35.253 1.00 63.53 **ATOM** 385 CA ASP 208 79.316 44.459 33.962 1.00 58.96 **ATOM** 386 CB ASP 208 78.746 43.434 32.974 1.00 62.84 **ATOM** 387 CG ASP 208 79.743 42.336 32.633 1.00 64.73 **ATOM** 388 OD1 ASP 208 79.575 41.200 33.121 1.00 66.65 **ATOM** 389 OD2 ASP 208 80.701 42.610 31.878 1.00 68.91 **ATOM** 390 C ASP 208 78.368 45.646 34.110 1.00 56.65 **ATOM** 391 O **ASP** 208 77.182 45.473 34.392 1.00 55.79 **ATOM** 392 N LYS 209 78.911 46.852 33.953 1.00 54.66 **ATOM** 393 CA LYS 209 78.132 48.081 34.082 1.00 53.92 **ATOM** 394 CB LYS 209 79.034 49.236 34.515 1.00 49.71 **ATOM** 395 C LYS 209 77.395 48.420 32.785 1.00 48.30 **ATOM** 396 O LYS 209 77.767 47.945 31.711 1.00 45.62 **ATOM** 397 N VAL 210 76.367 49.258 32.894 1.00 43.87 **ATOM** 398 CA VAL 210 75.539 49.662 31.757 1.00 41.25 **ATOM** 399 CB VAL 210 74.020 49.624 32.125 1.00 32.99 **ATOM** 400 CG1 VAL 210 73.153 50.029 30.937 1.00 31.44 401 CG2 VAL **ATOM** 210 73.626 48.239 32.604 1.00 27.57 **ATOM** 402 C VAL 210 75.868 51.061 31.234 1.00 43.30 **ATOM** 403 O VAL 210 76.261 51.951 31.994 1.00 44.65 **ATOM** 404 N ASP 211 75.688 51.235 29.931 1.00 43.23 **ATOM** 405 CA ASP 211 75.906 52.498 29.240 1.00 40.62 **ATOM** 406 CB ASP 211 76.686 52.232 27.943 1.00 43.49 **ATOM** 407 CG ASP 211 77.014 53.499 27.161 1.00 40.77 **ATOM** 408 OD1 ASP 211 76.180 54.427 27.092 1.00 42.13 **ATOM** 409 OD2 ASP 211 78.111 53.549 26.574 1.00 37.49 **ATOM** ASP 410 C 211 74.491 53.001 28.921 1.00 44.56 **ATOM** ASP 211 411 O 73.849 52.500 27.998 1.00 46.44 **ATOM** 412 N LEU 212 74.006 53.982 29.684 1.00 43.76 **ATOM** 413 CA LEU 212 72.662 54.538 29.494 1.00 41.47 **ATOM** 414 CB LEU 212 72.473 55.785 30.359 1.00 40.45 **ATOM** 415 CG LEU 212 72.360 55.585 31.867 1.00 44.47 **ATOM** 416 CD1 LEU 212 72.127 56.923 32.551 1.00 40.49 **ATOM** 417 CD2 LEU 212 71.217 54.634 32.153 1.00 45.94 **ATOM** 418 C LEU 212 72.325 54.886 28.049 1.00 40.77 **ATOM** 419 O LEU 212 71.254 54.540 27.548 1.00 42.25 **ATOM** 420 N GLU 213 73.241 55.588 27.394 1.00 42.53 **ATOM** 421 CA GLU 213 73.068 56.008 26.009 1.00 43.60 **ATOM** 422 CB GLU 213 74.267 56.860 25.598 1.00 43.84 **ATOM** 423 CG GLU 213 74.246 57.334 24.167 1.00 51.70 **ATOM** 424 CD GLU 213 75.598 57.848 23.722 1.00 59.23 **ATOM** 425 OE1 GLU 213 75.655 58.939 23.121 1.00 60.14 **ATOM** 426 OE2 GLU 76.611 57.158 23.980 1.00 64.78 213

ATOM 427 C GLU 213 72.913 54.810 25.066 1.00 42.63 428 O **ATOM** GLU 213 72.008 54.779 24.226 1.00 37.04 **ATOM** 429 N ALA 214 73.775 53.814 25.245 1.00 39.28 430 CA ALA 214 **ATOM** 73.753 52.605 24.424 1.00 39.52 **ATOM** 431 CB ALA 214 74.952 51.726 24.740 1.00 35.16 432 C ALA 214 **ATOM** 72.460 51.852 24.694 1.00 37.14 **ATOM** 433 O ALA 214 71.795 51.390 23.767 1.00 42.29 **ATOM** 434 N PHE 72.098 51.773 25.970 1.00 31.60 215 **ATOM** 435 CA PHE 215 70.883 51.102 26.404 1.00 31.67 **ATOM** 436 CB PHE 215 70.728 51.217 27.922 1.00 24.80 **ATOM** 437 CG PHE 215 69.512 50.522 28.458 1.00 21.78 **ATOM** 438 CD1 PHE 215 69.553 49.171 28.771 1.00 24.64 **ATOM** 439 CD2 PHE 215 68.328 51.223 28.658 1.00 21.53 **ATOM** 440 CE1 PHE 215 68.429 48.528 29.277 1.00 27.63 **ATOM** 441 CE2 PHE 215 67.200 50.591 29.163 1.00 21.60 **ATOM** 442 CZ PHE 215 67.249 49.242 29.472 1.00 21.35 ATOM 443 C PHE 215 69.675 51.706 25.694 1.00 35.75 **ATOM** 444 O PHE 215 68.838 50.975 25.161 1.00 34.84 **ATOM** 445 N SER 216 69.604 53.035 25.665 1.00 39.09 **ATOM** 446 CA SER 216 68.506 53.739 25.001 1.00 40.61 **ATOM** 447 CB SER 216 68.668 55.249 25.165 1.00 43.86 **ATOM** 448 OG SER 216 68.616 55.603 26.537 1.00 68.66 **ATOM** 449 C SER 216 68.444 53.380 23.518 1.00 40.76 **ATOM** 450 O SER 216 67.362 53.161 22.969 1.00 35.50 **ATOM** 451 N GLU 217 69.611 53.332 22.878 1.00 38.37 **ATOM** 452 CA GLU 217 69.709 52.989 21.462 1.00 37.80 **ATOM** 453 CB GLU 217 71.164 53.049 20.997 1.00 39.67 ATOM 454 CG GLU 217 71.701 54.461 20.880 1.00 46.65 **ATOM** 455 CD GLU 217 70.881 55.315 19.925 1.00 53.25 **ATOM** 456 OE1 GLU 217 70.920 55.056 18.702 1.00 57.12 **ATOM** 457 OE2 GLU 217 70.189 56.240 20.400 1.00 54.13 458 C GLU 217 **ATOM** 69.135 51.598 21.209 1.00 38.48 **ATOM** 459 O GLU 217 68.416 51.378 20.228 1.00 43.00 **ATOM** 460 N PHE 218 69.426 50.677 22.120 1.00 35.49 **ATOM** 461 CA PHE 218 68.934 49.313 22.018 1.00 31.76 **ATOM** 462 CB PHE 218 69.743 48.392 22.925 1.00 29.10 **ATOM** 463 CG PHE 218 71.169 48.260 22.510 1.00 26.25 **ATOM** 464 CD1 PHE 218 72.176 48.177 23.459 1.00 24.59 **ATOM** 465 CD2 PHE 71.510 48.233 21.163 1.00 23.53 218 **ATOM** 466 CE1 PHE 218 73.504 48.072 23.073 1.00 27.68 **ATOM** 467 CE2 PHE 218 72.832 48.128 20.765 1.00 25.37 **ATOM** 468 CZ PHE 218 73.834 48.047 21.721 1.00 28.43 **ATOM** 469 C PHE 218 67.445 49.202 22.321 1.00 31.30 **ATOM** 470 O PHE 218 66.726 48.496 21.621 1.00 35.18 **ATOM** 471 N THR 219 66.967 49.915 23.333 1.00 30.54 **ATOM** 472 CA THR 219 65.552 49.853 23.675 1.00 33.53 **ATOM** 473 CB THR 219 65.269 50.467 25.057 1.00 36.07

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ATOM	474 OG1 THR 219	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM	475 CG2 THR 219	65.797 49.562 26.145 1.00 34.32
ATOM	476 C THR 219	64.680 50.514 22.609 1.00 34.53
ATOM	477 O THR 219	63.507 50.162 22.450 1.00 36.57
ATOM	478 N LYS 220	65.267 51.457 21.873 1.00 38.13
ATOM	479 CA LYS 220	64.563 52.158 20.806 1.00 41.42
ATOM	480 CB LYS 220	65.452 53.257 20.208 1.00 41.62
ATOM	481 C LYS 220	64.140 51.182 19.716 1.00 41.80
ATOM	482 O LYS 220	63.032 51.274 19.192 1.00 43.29
ATOM	483 N ILE 221	65.018 50.234 19.393 1.00 36.93
ATOM	484 CA ILE 221	64.726 49.250 18.355 1.00 37.33
ATOM	485 CB ILE 221	65.965 48.932 17.482 1.00 33.71
ATOM	486 CG2 ILE 221	66.491 50.202 16.826 1.00 41.26
ATOM	487 CG1 ILE 221	67.042 48.235 18.309 1.00 30.36
ATOM	488 CD1 ILE 221	68.178 47.687 17.472 1.00 26.28
ATOM	489 C ILE 221	64.141 47.922 18.845 1.00 40.49
ATOM	490 O ILE 221	63.593 47.159 18.048 1.00 43.43
ATOM	491 N ILE 222	64.219 47.651 20.144 1.00 39.43
ATOM	492 CA ILE 222	63.703 46.394 20.667 1.00 35.49
ATOM	493 CB ILE 222	64.169 46.133 22.130 1.00 34.06
ATOM	494 CG2 ILE 222	63.287 46.881 23.130 1.00 26.15
ATOM	495 CG1 ILE 222	64.155 44.627 22.405 1.00 34.08
ATOM	496 CD1 ILE 222	64.760 44.220 23.719 1.00 33.67
ATOM	497 C ILE 222	62.186 46.230 20.539 1.00 37.60
ATOM	498 O ILE 222	61.703 45.127 20.279 1.00 42.14
ATOM	499 N THR 223	61.438 47.324 20.665 1.00 34.60
ATOM	500 CA THR 223	59.979 47.257 20.562 1.00 35.96
ATOM	501 CB THR 223	59.323 48.645 20.799 1.00 41.70
ATOM	502 OG1 THR 223	59.681 49.119 22.106 1.00 44.59
ATOM	503 CG2 THR 223	57.796 48.548 20.706 1.00 42.58
ATOM	504 C THR 223	59.478 46.614 19.252 1.00 34.77
ATOM	505 O THR 223	58.671 45.680 19.289 1.00 30.60
ATOM	506 N PRO 224	59.942 47.103 18.084 1.00 31.99
ATOM	507 CD PRO 224	60.784 48.288 17.839 1.00 30.37
ATOM	508 CA PRO 224	59.496 46.517 16.815 1.00 29.25
ATOM	509 CB PRO 224	60.225 47.366 15.769 1.00 29.27
ATOM	510 CG PRO 224	60.393 48.677 16.441 1.00 36.31
ATOM	511 C PRO 224	59.913 45.050 16.723 1.00 29.20
ATOM	512 O PRO 224	59.146 44.209 16.251 1.00 33.73
ATOM	513 N ALA 225	61.124 44.754 17.192 1.00 19.86
ATOM	514 CA ALA 225	61.663 43.395 17.175 1.00 19.61
ATOM	515 CB ALA 225	63.086 43.388 17.730 1.00 19.08
ATOM	516 C ALA 225	60.777 42.428 17.960 1.00 20.48
ATOM	517 O ALA 225	60.474 41.331 17.489 1.00 24.33
ATOM	518 N ILE 226	60.330 42.847 19.141 1.00 23.72
ATOM	519 CA ILE 226	59.471 42.001 19.972 1.00 21.94
ATOM	520 CB ILE 226	59.152 42.667 21.333 1.00 21.01
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ATOM	521 CG2 ILE 226	58.118 41.846 22.095 1.00 15.14
ATOM	522 CG1 ILE 226	60.425 42.841 22.163 1.00 20.45
ATOM	523 CD1 ILE 226	60.216 43.741 23.358 1.00 17.65
ATOM	524 C ILE 226	58.165 41.758 19.228 1.00 24.04
ATOM	525 O ILE 226	57.640 40.642 19.220 1.00 26.92
ATOM	526 N THR 227	57.653 42.811 18.596 1.00 25.22
ATOM	527 CA THR 227	56.410 42.730 17.836 1.00 27.92
ATOM	528 CB THR 227	55.984 44.132 17.333 1.00 34.33
ATOM	529 OG1 THR 227	55.823 45.007 18.458 1.00 33.62
ATOM	530 CG2 THR 227	54.669 44.061 16.563 1.00 39.18
ATOM	531 C THR 227	56.524 41.733 16.671 1.00 23.61
ATOM	532 O THR 227	55.587 40.977 16.413 1.00 24.41
ATOM	533 N ARG 228	57.670 41.704 15.995 1.00 15.49
ATOM	534 CA ARG 228	57.872 40.773 14.885 1.00 17.92
ATOM	535 CB ARG 228	59.174 41.075 14.137 1.00 19.84
ATOM	536 CG ARG 228	59.203 42.437 13.452 1.00 20.62
ATOM	537 CD ARG 228	60.351 42.523 12.453 1.00 24.29
ATOM	538 NE ARG 228	61.641 42.168 13.047 1.00 27.04
ATOM	539 CZ ARG 228	62.452 43.039 13.642 1.00 37.92
ATOM	540 NH1 ARG 228	62.113 44.327 13.725 1.00 42.82
ATOM	541 NH2 ARG 228	63.618 42.634 14.136 1.00 34.80
ATOM	542 C ARG 228	57.870 39.323 15.387 1.00 22.51
ATOM	543 O ARG 228	57.402 38.421 14.686 1.00 28.49
ATOM	544 N VAL 229	58.362 39.104 16.607 1.00 21.46
ATOM ATOM	545 CA VAL 229 546 CB VAL 229	58.372 37.762 17.187 1.00 20.12
ATOM	546 CB VAL 229 547 CG1 VAL 229	59.149 37.707 18.524 1.00 17.21 59.023 36.322 19.152 1.00 13.73
ATOM	548 CG2 VAL 229	60.611 38.019 18.287 1.00 15.80
ATOM	549 C VAL 229	56.926 37.348 17.421 1.00 19.19
ATOM	550 O VAL 229	56.528 36.224 17.089 1.00 19.86
ATOM	551 N VAL 230	56.134 38.275 17.953 1.00 21.49
ATOM	552 CA VAL 230	54.721 38.023 18.217 1.00 17.69
ATOM	553 CB VAL 230	54.041 39.239 18.881 1.00 21.30
ATOM	554 CG1 VAL 230	52.568 38.952 19.090 1.00 17.26
ATOM	555 CG2 VAL 230	54.706 39.572 20.218 1.00 17.13
ATOM	556 C VAL 230	54.003 37.707 16.902 1.00 26.39
ATOM	557 O VAL 230	53.180 36.790 16.843 1.00 29.63
ATOM	558 N ASP 231	54.333 38.451 15.848 1.00 25.52
ATOM	559 CA ASP 231	53.724 38.242 14.537 1.00 26.78
ATOM	560 CB ASP 231	54.132 39.353 13.571 1.00 23.70
ATOM	561 CG ASP 231	53.649 40.728 14.012 1.00 31.60
ATOM		52.656 40.820 14.771 1.00 31.79
ATOM	563 OD2 ASP 231	54.271 41.727 13.593 1.00 35.74
ATOM	564 C ASP 231	54.108 36.879 13.970 1.00 27.69
ATOM	565 O ASP 231	53.279 36.196 13.366 1.00 25.15
ATOM	566 N PHE 232	55.364 36.490 14.170 1.00 22.29
ATOM	567 CA PHE 232	55.858 35.200 13.703 1.00 23.78
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ATOM	568 CB PHE 232	57.328 35.008 14.097 1.00 24.76
ATOM	569 CG PHE 232	57.794 33.581 14.017 1.00 25.63
ATOM	570 CD1 PHE 232	58.000 32.967 12.785 1.00 24.50
ATOM	571 CD2 PHE 232	57.980 32.830 15.181 1.00 19.35
ATOM	572 CE1 PHE 232	58.381 31.630 12.705 1.00 22.27
ATOM	573 CE2 PHE 232	58.359 31.496 15.114 1.00 20.63
ATOM	574 CZ PHE 232	58.561 30.893 13.873 1.00 26.10
ATOM	575 C PHE 232	55.018 34.093 14.328 1.00 23.51
ATOM	576 O PHE 232	54.541 33.189 13.637 1.00 22.39
ATOM	577 N ALA 233	54.837 34.182 15.644 1.00 24.55
ATOM	578 CA ALA 233	54.070 33.192 16.387 1.00 23.10
ATOM	579 CB ALA 233	54.145 33.490 17.869 1.00 17.99
ATOM	580 C ALA 233	52.616 33.137 15.929 1.00 27.99
ATOM	581 O ALA 233	52.063 32.051 15.744 1.00 25.71
ATOM	582 N LYS 234	51.997 34.305 15.760 1.00 30.19
ATOM	583 CA LYS 234	50.601 34.380 15.325 1.00 31.58
ATOM	584 CB LYS 234	50.136 35.838 15.229 1.00 30.40
ATOM	585 CG LYS 234	50.100 36.593 16.555 1.00 37.97
ATOM	586 CD LYS 234	49.151 35.947 17.569 1.00 53.64
ATOM	587 CE LYS 234	47.694 35.958 17.101 1.00 59.60
ATOM	588 NZ LYS 234	46.773 35.268 18.060 1.00 54.22
ATOM	589 C LYS 234	50.388 33.686 13.978 1.00 30.35
ATOM	590 O LYS 234	49.318 33.142 13.716 1.00 32.50
ATOM	591 N LYS 235	51.425 33.687 13.144 1.00 23.98
ATOM	592 CA LYS 235	51.351 33.071 11.828 1.00 22.75
ATOM	593 CB LYS 235	52.353 33.737 10.896 1.00 23.12
ATOM	594 CG LYS 235	51.997 35.181 10.631 1.00 20.88
ATOM ATOM	595 CD LYS 235 596 CE LYS 235	52.982 35.836 9.688 1.00 26.50
ATOM	596 CE LYS 235 597 NZ LYS 235	52.512 37.227 9.310 1.00 31.33 53.439 37.862 8.341 1.00 36.51
ATOM	598 C LYS 235	
ATOM	599 O LYS 235	51.508 31.554 11.791 1.00 28.37 51.491 30.948 10.721 1.00 29.62
ATOM	600 N LEU 236	51.700 30.943 12.954 1.00 33.22
ATOM	601 CA LEU 236	51.828 29.494 13.036 1.00 32.24
ATOM	602 CB LEU 236	52.911 29.101 14.043 1.00 26.25
ATOM	603 CG LEU 236	54.327 29.582 13.730 1.00 23.40
ATOM	604 CD1 LEU 236	55.289 29.113 14.806 1.00 20.52
ATOM	605 CD2 LEU 236	54.750 29.054 12.374 1.00 20.29
ATOM	606 C LEU 236	50.470 28.984 13.502 1.00 37.08
ATOM	607 O LEU 236	50.013 29.342 14.588 1.00 34.23
ATOM	608 N PRO 237	49.811 28.134 12.695 1.00 44.89
ATOM	609 CD PRO 237	50.351 27.597 11.432 1.00 42.95
ATOM	610 CA PRO 237	48.491 27.556 12.990 1.00 48.88
ATOM	611 CB PRO 237	48.396 26.406 11.987 1.00 51.40
ATOM	612 CG PRO 237	49.142 26.931 10.813 1.00 53.54
ATOM	613 C PRO 237	48.278 27.072 14.430 1.00 49.12
ATOM	614 O PRO 237	47.387 27.551 15.133 1.00 48.18
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ATOM	615 N MET 238	49.104 26.126 14.860 1.00 45.79
ATOM	616 CA MET 238	49.029 25.558 16.200 1.00 52.79
ATOM	617 CB MET 238	50.133 24.505 16.378 1.00 49.72
ATOM	618 CG MET 238	49.861 23.195 15.637 1.00 58.16
ATOM	619 SD MET 238	51.342 22.205 15.284 1.00 60.11
ATOM	620 CE MET 238	50.993 21.626 13.625 1.00 53.03
ATOM	621 C MET 238	49.103 26.593 17.324 1.00 53.36
ATOM	622 O MET 238	48.583 26.365 18.420 1.00 58.87
ATOM	623 N PHE 239	49.713 27.742 17.043 1.00 48.09
ATOM	624 CA PHE 239	49.861 28.793 18.045 1.00 41.38
ATOM	625 CB PHE 239	51.011 29.736 17.677 1.00 32.92
ATOM	626 CG PHE 239	51.307 30.763 18.734 1.00 31.32
ATOM	627 CD1 PHE 239	52.162 30.462 19.790 1.00 28.28
ATOM	628 CD2 PHE 239	50.715 32.024 18.689 1.00 24.80
ATOM	629 CE1 PHE 239	52.425 31.402 20.790 1.00 29.45
ATOM	630 CE2 PHE 239	50.970 32.973 19.682 1.00 32.29
ATOM	631 CZ PHE 239	51.828 32.659 20.737 1.00 26.00
ATOM	632 C PHE 239	48.590 29.592 18.344 1.00 37.40
ATOM	633 O PHE 239	48.194 29.696 19.501 1.00 33.32
ATOM	634 N SER 240	47.958 30.166 17.321 1.00 36.32
ATOM	635 CA SER 240	46.745 30.959 17.529 1.00 39.00
ATOM	636 CB SER 240	46.385 31.724 16.258 1.00 47.52
ATOM	637 OG SER 240	47.390 32.671 15.947 1.00 52.67
ATOM	638 C SER 240	45.539 30.158 18.032 1.00 36.82
ATOM	639 O SER 240	44.548 30.743 18.485 1.00 43.02
ATOM	640 N GLU 241	45.617 28.833 17.931 1.00 38.98
ATOM	641 CA GLU 241	44.554 27.954 18.408 1.00 40.35
ATOM	642 CB GLU 241	44.788 26.521 17.926 1.00 49.38
ATOM	643 CG GLU 241 644 CD GLU 241	44.541 26.287 16.452 1.00 65.25
ATOM ATOM	644 CD GLU 241 645 OE1 GLU 241	44.873 24.856 16.002 1.00 70.72 44.806 23.923 16.845 1.00 73.36
ATOM	646 OE2 GLU 241	45.211 24.679 14.805 1.00 68.60
ATOM	647 C GLU 241	44.550 27.968 19.934 1.00 37.83
ATOM	648 O GLU 241	43.504 27.857 20.570 1.00 40.77
ATOM	649 N LEU 242	45.747 28.103 20:498 1.00 34.71
ATOM	650 CA LEU 242	45.974 28.132 21.944 1.00 31.77
ATOM	651 CB LEU 242	47.478 28.240 22.215 1.00 24.87
ATOM	652 CG LEU 242	48.345 27.006 22.455 1.00 30.51
ATOM	653 CD1 LEU 242	47.814 25.763 21.772 1.00 31.72
ATOM	654 CD2 LEU 242	49.743 27.328 21.996 1.00 24.25
ATOM	655 C LEU 242	45.274 29.287 22.657 1.00 29.41
ATOM	656 O LEU 242	45.029 30.339 22.071 1.00 28.12
ATOM	657 N PRO 243	44.913 29.089 23.938 1.00 32.37
ATOM	658 CD PRO 243	44.976 27.849 24.728 1.00 27.94
ATOM	659 CA PRO 243	44.253 30.165 24.685 1.00 33.92
ATOM	660 CB PRO 243	44.041 29.537 26.065 1.00 29.41
ATOM	661 CG PRO 243	43.929 28.072 25.775 1.00 30.77

ATOM 662 C **PRO** 243 45.246 31.334 24.775 1.00 35.86 **ATOM** 663 O **PRO** 243 46.461 31.110 24.809 1.00 38.79 **ATOM** 664 N **CYS** 244 44.751 32.570 24.834 1.00 39.67 **ATOM** 665 CA CYS 244 45.621 33.749 24.931 1.00 45.78 **ATOM** 666 CB CYS 244 44.788 35.028 25.102 1.00 71.13 **ATOM** 667 SG CYS 244 44.068 35.680 23.580 1.00100.76 **ATOM** 669 C CYS 244 46.660 33.665 26.051 1.00 40.08 **ATOM** 670 O **CYS** 244 47.797 34.096 25.879 1.00 35.68 **ATOM** 671 N GLU 245 46.265 33.088 27.184 1.00 34.25 **ATOM** 672 CA GLU 245 47.156 32.939 28.337 1.00 34.60 **ATOM** 673 CB GLU 245 46.426 32.296 29.524 1.00 42.20 **ATOM** 674 CG GLU 245 45.356 33.171 30.160 1.00 41.92 **ATOM** 675 CD GLU 245 43.947 32.808 29.730 1.00 39.68 **ATOM** 676 OE1 GLU 245 43.080 32.693 30.618 1.00 38.31 **ATOM** 677 OE2 GLU 245 43.697 32.644 28.516 1.00 48.13 **ATOM** 678 C GLU 245 48.376 32.109 27.984 1.00 29.54 **ATOM** 679 O GLU 245 49.497 32.437 28.381 1.00 33.54 680 N ASP **ATOM** 246 48.146 31.034 27.236 1.00 26.40 246 **ATOM** 681 CA ASP 49.219 30.154 26.794 1.00 26.99 682 CB ASP 48.650 28.887 26.153 1.00 29.86 **ATOM** 246 **ATOM** 683 CG ASP 246 48.184 27.876 27.175 1.00 34.10 **ATOM** 684 OD1 ASP 246 48.149 28.199 28.381 1.00 31.83 **ATOM** 685 OD2 ASP 246 47.863 26.742 26.772 1.00 35.79 **ATOM** 686 C ASP 246 50.103 30.875 25.790 1.00 28.07 **ATOM** 687 O ASP 246 51.331 30.789 25.863 1.00 27.35 **ATOM** 688 N GLN 247 49.472 31.577 24.851 1.00 25.53 **ATOM** 689 CA GLN 247 50.198 32.327 23.829 1.00 26.08 **ATOM** 690 CB GLN 247 49.228 33.089 22.924 1.00 23.38 **ATOM** 691 CG GLN 247 48.303 32.213 22.091 1.00 23.76 **ATOM** 692 CD GLN 247 47.429 33.029 21.151 1.00 26.89 **ATOM** 693 OE1 GLN 247 47.853 34.054 20.628 1.00 33.51 **ATOM** 694 NE2 GLN 247 46.198 32.593 20.957 1.00 27.44 **ATOM** 695 C GLN 247 51.133 33.313 24.511 1.00 22.74 **ATOM** 696 O GLN 247 52.326 33.373 24.205 1.00 27.63 **ATOM** 697 N ILE 248 50.588 34.047 25.473 1.00 25.03 698 CA ILE 248 51.353 35.035 26.220 1.00 25.94 **ATOM** 699 CB ILE 248 50.436 35.781 27.226 1.00 24.84 **ATOM ATOM** 700 CG2 ILE 248 51.251 36.633 28.179 1.00 21.87 701 CG1 ILE 248 **ATOM** 49.430 36.652 26.459 1.00 27.98 **ATOM** 702 CD1 ILE 248 48.359 37.298 27.328 1.00 29.90 **ATOM** 703 C ILE 248 52.535 34.382 26.939 1.00 27.53 **ATOM** 704 O ILE 248 53.671 34.847 26.833 1.00 29.35 705 N ILE 249 52.279 33.274 27.622 1.00 24.38 **ATOM** 706 CA ILE 249 **ATOM** 53.334 32.582 28.354 1.00 26.26 **ATOM** 707 CB ILE 249 52.759 31.395 29.166 1.00 29.81 708 CG2 ILE 249 **ATOM** 53.874 30.521 29.726 1.00 29.16 **ATOM** 709 CG1 ILE 249 51.883 31.923 30.300 1.00 27.15

ATOM 710 CD1 ILE 249 51.173 30.838 31.076 1.00 32.35 **ATOM** 711 C ILE 249 54.448 32.103 27.422 1.00 27.78 **ATOM** 712 O ILE 249 55.634 32.297 27.708 1.00 29.37 **ATOM** 713 N LEU 250 54.061 31.516 26.289 1.00 29.25 **ATOM** 714 CA LEU 250 55.021 31.005 25.319 1.00 24.49 **ATOM** 715 CB LEU 250 54.303 30.224 24.214 1.00 23.75 **ATOM** 716 CG LEU 250 53.541 28.962 24.629 1.00 23.18 **ATOM** 717 CD1 LEU 250 52.886 28.353 23.416 1.00 19.94 **ATOM** 718 CD2 LEU 250 54.475 27.960 25.278 1.00 20.76 **ATOM** 719 C LEU 250 55.878 32.116 24.714 1.00 22.20 **ATOM** 720 O LEU 250 57.082 31.940 24.528 1.00 23.49 **ATOM** 721 N LEU 251 55.256 33.249 24.399 1.00 24.21 **ATOM 722 CA LEU** 251 55.980 34.384 23.831 1.00 27.98 **ATOM 723 CB LEU** 251 55.010 35.488 23.408 1.00 25.91 **ATOM** 724 CG LEU 251 54.287 35.245 22.085 1.00 29.46 **ATOM** 725 CD1 LEU 251 53.121 36.217 21.939 1.00 35.03 **ATOM** 726 CD2 LEU 251 55.268 35.364 20.924 1.00 23.65 **ATOM** 727 C LEU 251 56.998 34.931 24.828 1.00 26.85 **ATOM** 728 O LEU 251 58.165 35.143 24.484 1.00 23.12 **ATOM** 729 N LYS 252 56.556 35.145 26.063 1.00 25.33 57.427 35.644 27.119 1.00 31.33 **ATOM** 730 CA LYS 252 **ATOM** 731 CB LYS 252 56.659 35.723 28.437 1.00 37.06 **ATOM** 732 CG LYS 252 55.593 36.805 28.511 1.00 41.75 **ATOM** 733 CD LYS 252 54.779 36.619 29.783 1.00 52.64 **ATOM** 734 CE LYS 252 53.822 37.767 30.057 1.00 62.60 252 **ATOM** 735 NZ LYS 54.503 39.005 30.520 1.00 71.68 **ATOM** 736 C LYS 252 58.622 34.705 27.293 1.00 29.08 **ATOM** 737 O LYS 252 59.758 35.150 27.460 1.00 35.24 738 N GLY **ATOM** 253 58.355 33.403 27.211 1.00 24.98 **739 CA GLY** 253 **ATOM** 59.407 32.416 27.369 1.00 22.80 ATOM 740 C GLY 253 60.413 32.282 26.235 1.00 26.90 **ATOM** 741 O **GLY** 253 61.572 31.948 26.489 1.00 31.90 742 N CYS 254 **ATOM** 60.013 32.574 24.997 1.00 25.42 **ATOM** 743 CA CYS 254 60.932 32.427 23.863 1.00 20.71 **ATOM** 744 CB CYS 254 60.314 31.509 22.811 1.00 24.98 **ATOM** 745 SG CYS 254 58.976 32.310 21.909 1.00 24.24 **ATOM** 746 C CYS 254 61.353 33.716 23.164 1.00 22.79 CYS 254 **ATOM** 747 O 62.217 33.683 22.282 1.00 23.23 **ATOM** 748 N CYS 255 60.757 34.842 23.539 1.00 21.47 **ATOM** 749 CA CYS 255 61.061 36.114 22.884 1.00 22.50 750 CB CYS 255 **ATOM** 60.318 37.262 23.567 1.00 21.72 **ATOM 751 SG CYS** 255 60.353 38.768 22.597 1.00 24.73 **ATOM** 752 C **CYS** 255 62.547 36.457 22.738 1.00 23.81 **CYS** 255 **ATOM** 753 O 63.015 36.746 21.632 1.00 23.48 **ATOM MET** 256 754 N 63.294 36.402 23.838 1.00 22.13 **ATOM 755 CA MET** 256 64.719 36.713 23.792 1.00 22.91 65.286 36.810 25.213 1.00 23.78 **ATOM 756 CB MET** 256

ATOM	757 CG MET 256	66.781 37.094 25.272 1.00 17.41
ATOM	758 SD MET 256	67.196 38.632 24.415 1.00 23.65
ATOM	759 CE MET 256	69.010 38.715 24.624 1.00 18.57
ATOM	760 C MET 256	65.487 35.671 22.980 1.00 21.41
ATOM	761 O MET 256	66.432 36.005 22.260 1.00 22.01
ATOM	762 N · GLU 257	65.058 34.415 23.068 1.00 23.18
ATOM	763 CA GLU 257	65.705 33.323 22.345 1.00 22.90
ATOM	764 CB GLU 257	65.085 31.989 22.753 1.00 24.00
ATOM	765 CG GLU 257	65.522 31.521 24.125 1.00 33.44
ATOM	766 CD GLU 257	64.564 30.527 24.735 1.00 38.03
ATOM	767 OE1 GLU 257	63.977 29.705 24.000 1.00 45.59
ATOM	768 OE2 GLU 257	64.385 30.577 25.965 1.00 45.75
ATOM	769 C GLU 257	65.595 33.526 20.840 1.00 21.68
ATOM	770 O GLU 257	66.586 33.421 20.107 1.00 20.02
ATOM	771 N ILE 258	64.383 33.852 20.391 1.00 17.07
ATOM	772 CA ILE 258	64.135 34.090 18.973 1.00 17.01
ATOM	773 CB ILE 258	62.613 34.207 18.684 1.00 17.33
ATOM	774 CG2 ILE 258	62.369 34.758 17.276 1.00 15.91
ATOM	775 CG1 ILE 258	61.952 32.831 18.885 1.00 16.69
ATOM	776 CD1 ILE 258	60.450 32.783 18.632 1.00 16.31
ATOM	777 C ILE 258	64.911 35.324 18.501 1.00 17.65
ATOM	778 O ILE 258	65.605 35.263 17.484 1.00 22.58
ATOM	779 N MET 259	64.865 36.410 19.274 1.00 20.17
ATOM	780 CA MET 259	65.584 37.628 18.909 1.00 15.03
ATOM ATOM	781 CB MET 259 782 CG MET 259	65.234 38.771 19.856 1.00 20.12
ATOM	783 SD MET 259	63.791 39.191 19.775 1.00 17.19 63.523 40.795 20.524 1.00 28.92
ATOM	784 CE MET 259	63.523 40.795 20.524 1.00 28.92 63.718 40.406 22.261 1.00 19.58
ATOM	785 C MET 259	67.090 37.402 18.884 1.00 18.84
ATOM	786 O MET 259	67.783 37.912 17.996 1.00 29.07
ATOM	787 N SER 260	67.590 36.618 19.837 1.00 21.45
ATOM	788 CA SER 260	69.019 36.319 19.906 1.00 18.71
ATOM	789 CB SER 260	69.367 35.595 21.207 1.00 18.35
ATOM	790 OG SER 260	69.128 36.421 22.329 1.00 25.42
ATOM	791 C SER 260	69.430 35.469 18.709 1.00 17.83
ATOM	792 O SER 260	70.497 35.673 18.131 1.00 22.97
ATOM	793 N LEU 261	68.572 34.522 18.331 1.00 21.66
ATOM	794 CA LEU 261	68.837 33.663 17.179 1.00 20.98
ATOM	795 CB LEU 261	67.739 32.608 17.053 1.00 22.66
ATOM	796 CG LEU 261	67.719 31.759 15.781 1.00 22.12
ATOM	797 CD1 LEU 261	68.998 30.938 15.665 1.00 18.51
ATOM	798 CD2 LEU 261	66.498 30.851 15.800 1.00 19.60
ATOM	799 C LEU 261	68.873 34.527 15.920 1.00 22.95
ATOM	800 O LEU 261	69.779 34.402 15.091 1.00 22.62
ATOM	801 N ARG 262	67.892 35.418 15.798 1.00 22.12
ATOM	802 CA ARG 262	67.816 36.301 14.643 1.00 25.32
ATOM	803 CB ARG 262	66.525 37.115 14.677 1.00 21.95

ATOM	804 CG ARG 262	65.304 36.268 14.362 1.00 21.48
ATOM	805 CD ARG 262	64.026 37.077 14.345 1.00 19.12
ATOM	806 NE ARG 262	62.990 36.377 13.599 1.00 22.18
ATOM	807 CZ ARG 262	61.780 36.862 13.333 1.00 22.88
ATOM	808 NH1 ARG 262	
ATOM	809 NH2 ARG 262	60.912 36.129 12.648 1.00 20.26
ATOM	810 C ARG 262	69.044 37.196 14.531 1.00 25.05
ATOM	811 O ARG 262	69.485 37.513 13.427 1.00 22.98
ATOM	812 N ALA 263	69.608 37.579 15.676 1.00 26.36
ATOM	813 CA ALA 263	70.818 38.400 15.705 1.00 27.02
ATOM	814 CB ALA 263	70.997 39.045 17.087 1.00 25.80
ATOM	815 C ALA 263	72.026 37.514 15.368 1.00 25.21
ATOM	816 O ALA 263	72.825 37.844 14.492 1.00 31.14
ATOM	817 N ALA 264	72.109 36.358 16.027 1.00 25.62
ATOM	818 CA ALA 264	73.203 35.408 15.828 1.00 23.85
ATOM	819 CB ALA 264	73.062 34.237 16.794 1.00 17.15
ATOM	820 C ALA 264	73.345 34.901 14.391 1.00 26.03
ATOM	821 O ALA 264	74.460 34.773 13.886 1.00 25.66
ATOM	822 N VAL 265	72.234 34.615 13.723 1.00 25.22
ATOM	823 CA VAL 265	72.327 34.128 12.350 1.00 28.38
ATOM	824 CB VAL 265	71.028 33.457 11.857 1.00 24.59
ATOM	825 CG1 VAL 265	70.707 32.264 12.719 1.00 25.53
ATOM	826 CG2 VAL 265	69.881 34.440 11.853 1.00 20.86
ATOM	827 C VAL 265	72.747 35.235 11.393 1.00 31.46
ATOM	828 O VAL 265	73.024 34.973 10.222 1.00 34.75
ATOM	829 N ARG 266	72.795 36.464 11.896 1.00 30.10
ATOM ATOM	830 CA ARG 266	73.211 37.602 11.089 1.00 30.69
ATOM	831 CB ARG 266 832 CG ARG 266	72.170 38.713 11.148 1.00 25.13
ATOM	832 CG ARG 266 833 CD ARG 266	70.976 38.406 10.299 1.00 25.43
ATOM	834 NE ARG 266	69.999 39.537 10.277 1.00 29.56 69.032 39.340 9.205 1.00 31.59
ATOM	835 CZ ARG 266	69.032 39.340 9.205 1.00 31.59 67.814 39.861 9.197 1.00 31.18
ATOM	836 NH1 ARG 266	67.408 40.611 10.215 1.00 31.18
ATOM	837 NH2 ARG 266	67.012 39.648 8.163 1.00 28.21
ATOM	838 C ARG 266	74.568 38.111 11.544 1.00 34.28
ATOM	839 O ARG 266	74.877 39.300 11.423 1.00 41.19
ATOM	840 N TYR 267	75.362 37.207 12.108 1.00 30.80
ATOM	841 CA TYR 267	76.694 37.544 12.573 1.00 33.84
ATOM	842 CB TYR 267	77.202 36.461 13.534 1.00 32.56
ATOM	843 CG TYR 267	78.674 36.570 13.867 1.00 34.23
ATOM	844 CD1 TYR 267	79.131 37.465 14.835 1.00 32.60
ATOM	845 CE1 TYR 267	80.491 37.593 15.106 1.00 34.90
ATOM	846 CD2 TYR 267	79.615 35.801 13.184 1.00 32.84
ATOM	847 CE2 TYR 267	80.972 35.920 13.446 1.00 34.70
ATOM	848 CZ TYR 267	81.404 36.816 14.405 1.00 36.21
ATOM	849 OH TYR 267	82.749 36.940 14.651 1.00 39.48
ATOM	850 C TYR 267	77.615 37.649 11.360 1.00 37.82
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ATOM 851 O **TYR** 267 77.648 36.749 10.517 1.00 39.45 **ATOM** 852 N **ASP** 268 78.319 38.769 11.239 1.00 44.62 **ATOM** 853 CA ASP 268 79.248 38.963 10.133 1.00 45.56 **ATOM** 854 CB ASP 268 79.096 40.366 9.533 1.00 46.62 **ATOM** 855 CG ASP 268 80.068 40.624 8.391 1.00 50.96 **ATOM** 856 OD1 ASP 268 80.204 39.755 7.502 1.00 55.65 857 OD2 ASP ATOM 268 80.700 41.699 8.384 1.00 52.09 **ATOM** 858 C **ASP** 268 80.675 38.751 10.630 1.00 44.44 **ATOM** 859 O **ASP** 268 81.242 39.614 11.304 1.00 45.68 **ATOM** 860 N PRO 269 81.281 37.600 10.296 1.00 45.94 **ATOM** 861 CD PRO 269 80.739 36.503 9.476 1.00 43.72 **ATOM** 862 CA PRO 269 82.651 37.309 10.730 1.00 46.63 ATOM 863 CB PRO 269 82.884 35.889 10.208 1.00 43.88 **ATOM** 864 CG PRO 269 81.983 35.797 9.018 1.00 44.66 **ATOM** 865 C PRO 269 83.682 38.298 10.190 1.00 50.80 **ATOM** 866 O **PRO** 269 84.681 38.578 10.854 1.00 48.56 **ATOM** 867 N **ALA** 270 9.012 1.00 55.09 83.407 38.858 **ATOM** 868 CA ALA 270 84.306 39.820 8.374 1.00 55.68 **ATOM** 869 CB ALA 270 83.799 40.168 6.974 1.00 53.64 **ATOM** 870 C ALA 270 84.528 41.096 9.196 1.00 56.18 **ATOM** 871 O ALA 270 85.577 41.729 9.082 1.00 61.07 **ATOM** 872 N SER 271 83.543 41.479 10.006 1.00 51.38 **ATOM** 873 CA SER 271 83.661 42.678 10.836 1.00 45.90 **ATOM** 874 CB SER 271 82.710 43.774 10.346 1.00 44.49 **ATOM** 875 OG SER 271 81.360 43.358 10.404 1.00 45.26 **ATOM** 876 C SER 271 83.409 42.395 12.317 1.00 46.61 **ATOM** 877 O SER 271 83.431 43.309 13.143 1.00 48.31 **ATOM** 878 N **ASP** 272 83.172 41.126 12.642 1.00 46.73 **ATOM** 879 CA ASP 272 82.920 40.689 14.013 1.00 42.49 **ATOM** 880 CB ASP 272 84.200 40.807 14.849 1.00 42.12 **ATOM** 881 CG ASP 272 84.103 40.072 16.169 1.00 50.30 **ATOM** 272 882 OD1 ASP 83.417 39.028 16.218 1.00 45.10 **ATOM** 883 OD2 ASP 272 84.708 40.537 17.160 1.00 57.61 **ATOM** 884 C **ASP** 272 81.769 41.465 14.658 1.00 40.95 **ATOM** 885 O **ASP** 272 81.885 41.975 15:779 1.00 42.93 **ATOM** 886 N THR 273 80.651 41.531 13.945 1.00 38.57 **ATOM** 887 CA THR 273 79.473 42.239 14.425 1.00 40.99 **ATOM** 888 CB THR 273 79.262 43.574 13.656 1.00 40.76 273 **ATOM** 889 OG1 THR 79.240 43.318 12.248 1.00 42.61 **ATOM** 890 CG2 THR 273 80.373 44.574 13.965 1.00 39.67 **ATOM** 891 C THR 273 78.210 41.397 14.251 1.00 39.94 THR **ATOM** 892 O 273 78.202 40.419 13.494 1.00 36.66 **ATOM** 893 N LEU 274 77.168 41.757 14.993 1.00 36.08 **ATOM** 894 CA LEU 274 75.867 41.096 14.907 1.00 34.28 **ATOM** 895 CB LEU 274 75.343 40.699 16.292 1.00 30.96 **ATOM** 896 CG LEU 274 75.952 39.536 17.068 1.00 30.19 **ATOM** 897 CD1 LEU 274 75.310 39.472 18.444 1.00 26.29

ATOM 898 CD2 LEU 274 75.744 38.237 16.309 1.00 27.43 ATOM 899 C LEU 274 74.943 42.163 14.347 1.00 36.49 **ATOM** 900 O LEU 274 75.152 43.354 14.596 1.00 40.27 **ATOM** 901 N THR 275 73.923 41.758 13.606 1.00 36.42 **ATOM** 902 CA THR 275 72.994 42.731 13.062 1.00 35.07 **ATOM** 903 CB THR 275 72.773 42.522 11.556 1.00 36.04 **ATOM** 904 OG1 THR 275 74.028 42.625 10.875 1.00 41.52 **ATOM** 905 CG2 THR 275 71.852 43.583 11.008 1.00 36.47 **ATOM** 906 C THR 275 71.673 42.655 13.814 1.00 34.32 **ATOM** 907 O THR 275 71.055 41.590 13.907 1.00 34.96 **ATOM** 908 N LEU 276 71.292 43.767 14.432 1.00 31.79 ATOM 909 CA LEU 276 70.044 43.840 15.173 1.00 29.47 **ATOM** 910 CB LEU 276 70.181 44.766 16.389 1.00 25.29 **ATOM** 911 CG LEU 276 71.328 44.501 17.383 1.00 29.01 **ATOM** 912 CD1 LEU 276 71.179 45.410 18.594 1.00 20.92 **ATOM** 913 CD2 LEU 276 71.358 43.042 17.834 1.00 22.79 **ATOM** 914 C LEU 276 68.966 44.350 14.228 1.00 31.69 LEU 276 **ATOM** 915 O 69.175 45.335 13.510 1.00 33.87 **ATOM** 916 N SER 277 67.862 43.608 14.162 1.00 33.07 **ATOM** 917 CA SER 277 66.721 43.935 13.315 1.00 30.61 **ATOM** 918 CB SER 277 65.949 45.111 13.909 1.00 22.87 277 **ATOM** 919 OG SER 65.587 44.822 15.250 1.00 23.35 **ATOM** 920 C SER 277 67.103 44.200 11.860 1.00 31.85 277 **ATOM** 921 O SER 66.433 44.958 11.158 1.00 32.13 **ATOM** 922 N GLY 278 68.188 43.566 11.421 1.00 32.29 **ATOM** 923 CA GLY 278 68.664 43.716 10.058 1.00 37.59 69.063 45.122 9.639 1.00 43.26 **ATOM** 924 C GLY 278 **ATOM** 925 O GLY 278 69.313 45.358 8.455 1.00 42.60 279 **ATOM** 926 N GLU 69.177 46.038 10.599 1.00 43.42 **ATOM** 927 CA GLU 279 69.532 47.420 10.291 1.00 44.55 **ATOM** 928 CB GLU 279 68.292 48.310 10.394 1.00 44.66 **ATOM** 929 CG GLU 279 67.671 48.344 11.783 1.00 54.19 279 **ATOM** 930 CD GLU 66.400 49.171 11.845 1.00 64.96 **ATOM** 279 931 OE1 GLU 65.627 49.174 10.859 1.00 71.43 932 OE2 GLU 279 **ATOM** 66.167 49.814 12.891 1.00 66.65 933 C GLU 279 **ATOM** 70.654 48.019 11.133 1.00 45.52 **ATOM** 934 O GLU 279 71.207 49.057 10.772 1.00 51.83 **ATOM** 935 N MET 280 71.007 47.373 12.242 1.00 44.66 **936 CA MET** 280 72.060 47.904 13.105 1.00 34.22 **ATOM ATOM 937 CB MET** 280 71.470 48.382 14.433 1.00 32.38 **ATOM** 938 CG MET 280 72.479 49.058 15.345 1.00 37.87 **ATOM** 939 SD MET 280 71.912 49.201 17.052 1.00 41.78 **ATOM** 940 CE MET 280 70.650 50.495 16.911 1.00 37.01 **ATOM** 941 C **MET** 280 73.183 46.920 13.386 1.00 35.70 280 **ATOM** 942 O **MET** 72.976 45.900 14.044 1.00 36.99 **ATOM** 943 N **ALA** 281 74.366 47.221 12.867 1.00 34.80 **ATOM** 944 CA ALA 281 75.535 46.377 13.091 1.00 35.11

ATOM 945 CB ALA 281 76.529 46.527 11.955 1.00 31.27 **ATOM** 946 C ALA 281 76.155 46.837 14.406 1.00 35.96 **ATOM** 947 O ALA 281 76.478 48.015 14.570 1.00 39.10 948 N VAL **ATOM** 282 76.285 45.916 15.353 1.00 36.46 **ATOM** 949 CA VAL 282 76.839 46.246 16.655 1.00 36.05 **ATOM** 950 CB VAL 282 75.783 46.090 17.783 1.00 35.60 951 CG1 VAL 282 **ATOM** 74.633 47.069 17.568 1.00 38.73 **ATOM** 952 CG2 VAL 282 75.262 44.660 17.844 1.00 33.27 **ATOM** 953 C VAL 282 78.062 45.408 16.996 1.00 37.70 **ATOM** 954 O VAL 282 78.137 44.223 16.660 1.00 37.45 **ATOM** 955 N 283 ALA 79.032 46.047 17.637 1.00 39.21 956 CA ALA 283 **ATOM** 80.254 45.375 18.048 1.00 43.73 **ATOM** 957 CB ALA 283 81.433 46.352 18.047 1.00 42.04 **ATOM** 958 C ALA 283 80.060 44.752 19.435 1.00 43.28 **ATOM** 959 O ALA 283 79.179 45.157 20.203 1.00 45.77 **ATOM** 960 N ARG 284 80.903 43.774 19.744 1.00 41.96 **ATOM** 961 CA ARG 284 80.866 43.044 21.004 1.00 44.87 **ATOM** 962 CB ARG 284 82.084 42.125 21.087 1.00 46.34 **ATOM** 963 CG ARG 284 81.930 40.947 22.017 1.00 51.85 **ATOM** 964 CD ARG 284 83.107 40.010 21.844 1.00 60.73 **ATOM** 965 NE ARG 284 83.262 39.571 20.455 1.00 54.30 **ATOM** 966 CZ ARG 284 83.221 38.300 20.074 1.00 53.66 **ATOM** 967 NH1 ARG 284 83.032 37.343 20.973 1.00 49.99 **ATOM** 968 NH2 ARG 284 83.379 37.984 18.797 1.00 47.31 **ATOM** 969 C ARG 284 80.803 43.945 22.237 1.00 44.85 **ATOM** 970 O ARG 284 79.896 43.806 23.062 1.00 48.26 **ATOM** 971 N **GLU** 285 81.750 44.873 22.349 1.00 41.60 **ATOM** 972 CA GLU 285 81.802 45.787 23.484 1.00 41.17 **ATOM** 973 CB GLU 285 83.043 46.675 23.392 1.00 39.97 **ATOM** 974 C GLU 285 80.538 46.640 23.603 1.00 40.08 **ATOM** 975 O GLU 285 80.023 46.849 24.703 1.00 41.16 **ATOM** 976 N GLN 286 80.017 47.088 22.463 1.00 38.49 **ATOM** 977 CA GLN 286 78.818 47.926 22.425 1.00 36.25 ATOM 978 CB GLN 286 78.549 48.401 20.997 1.00 39.50 **ATOM** 979 CG GLN 286 79.619 49.311 20.424 1.00 43.62 **ATOM** 980 CD GLN 286 79.324 49.710 18.987 1.00 49.48 **ATOM** 981 OE1 GLN 286 79.253 48.856 18.097 1.00 48.41 **ATOM** 982 NE2 GLN 286 79.125 51.000 18.755 1.00 47.15 **ATOM** 983 C GLN 286 77.563 47.255 22.988 1.00 35.40 **ATOM** 984 O GLN 286 76.903 47.806 23.871 1.00 31.24 985 N LEU **ATOM** 287 77.234 46.071 22.480 1.00 32.96 **ATOM** 986 CA LEU 287 76.055 45.349 22.950 1.00 33.40 ATOM 987 CB LEU 287 75.767 44.138 22.054 1.00 28.67 **ATOM** 988 CG LEU 287 74.466 43.375 22.342 1.00 26.66 **ATOM** 989 CD1 LEU 287 73.263 44.305 22.244 1.00 19.41 **ATOM** 990 CD2 LEU 287 74.325 42.221 21.368 1.00 24.84 76.234 44.914 24.406 1.00 34.81 **ATOM** 991 C LEU 287

ATOM	992	O LEU	287	75.265 44.857 25.175 1.00 33.92
ATOM	993	N LYS	288	77.476 44.621 24.781 1.00 35.38
ATOM	994	CA LYS	288	77.814 44.204 26.140 1.00 36.12
ATOM	995	CB LYS	288	79.296 43.839 26.210 1.00 37.13
ATOM	996	CG LYS	288	79.762 43.280 27.533 1.00 44.61
ATOM	997	CD LYS	288	81.256 43.018 27.494 1.00 54.07
ATOM	998	CE LYS	288	81.757 42.435 28.801 1.00 60.87
ATOM	999	•	288	81.291 41.041 29.039 1.00 61.53
ATOM	1000		288	77.510 45.345 27.109 1.00 36.90
ATOM	1001		288	76.684 45.206 28.013 1.00 40.68
ATOM	1002		289	78.129 46.495 26.863 1.00 35.94
ATOM	1003			77.947 47.680 27.695 1.00 36.12
ATOM	1004		289	78.982 48.738 27.332 1.00 31.78
ATOM	1005			80.388 48.263 27.569 1.00 40.31
ATOM	1006			80.627 47.422 28.440 1.00 43.12
ATOM		ND2 ASN		81.326 48.758 26.775 1.00 35.36
ATOM			289	76.553 48.277 27.590 1.00 36.98
ATOM	1009		289	76.099 48.959 28.509 1.00 34.29
ATOM ATOM	1010 1011	N GLY CA GLY	290 290	75.883 48.032 26.466 1.00 32.65
ATOM	1011	CA GL1	290	74.541 48.550 26.256 1.00 28.61
ATOM	1012	O GLY	290	73.497 48.001 27.210 1.00 26.54 72.362 48.480 27.234 1.00 31.06
ATOM	1013	N GLY	291	73.861 46.978 27.977 1.00 28.89
ATOM		CA GLY		72.929 46.413 28.937 1.00 25.24
ATOM	1015	CA GLY	291	72.872 44.900 28.997 1.00 28.12
ATOM	1017	O GLY	291	72.335 44.345 29.955 1.00 31.16
ATOM	1018	N LEU	292	73.406 44.223 27.985 1.00 29.51
ATOM	1019	CA LEU	292	73.361 42.766 27.969 1.00 32.79
ATOM	1020	CB LEU	292	73.304 42.240 26.531 1.00 28.00
ATOM	1021	CG LEU	292	71.948 42.355 25.827 1.00 23.68
ATOM-	1022	CD1 LEU	292	72.004 41.626 24.509 1.00 26.12
ATOM	1023	CD2 LEU	292	70.851 41.764 26.694 1.00 23.36
ATOM	1024	C LEU	292	74.484 42.085 28.742 1.00 32.33
ATOM	1025	O LEU	292	74.312 40.967 29.232 1.00 32.22
ATOM	1026	N GLY	293	75.627 42.750 28.846 1.00 30.31
ATOM			293	76.751 42.176 29.561 1.00 28.82
ATOM	1028			77.238 40.894 28.913 1.00 29.87
ATOM		O GLY	293	77.432 40.843 27.698 1.00 35.43
ATOM		N VAL		77.392 39.848 29.714 1.00 31.88
ATOM			294	77.866 38.561 29.217 1.00 35.77
ATOM			294	78.232 37.590 30.363 1.00 34.29
ATOM		CG1 VAL	294	79.462 38.092 31.095 1.00 37.54
ATOM			294	77.065 37.425 31.322 1.00 25.62
ATOM			294	76.882 37.879 28.274 1.00 35.89
ATOM			294	77.263 36.960 27.541 1.00 37.99
ATOM			295	75.619 38.304 28.305 1.00 34.41
ATOM	1038	CA VAL	295	74.616 37.728 27.413 1.00 32.98

ATOM 1039 CB VAL 295 73.208 38.298 27.677 1.00 31.25 **ATOM** 1040 CG1 VAL 295 72.208 37.706 26.694 1.00 23.54 **ATOM** 1041 CG2 VAL 295. 72.783 37.993 29.101 1.00 23.07 **ATOM** 1042 C VAL 295 75.057 38.062 25.993 1.00 33.92 **ATOM** 1043 O VAL 295 74.932 37.238 25.090 1.00 36.95 ATOM 1044 N. SER 75.625 39.253 25.820 1.00 31.27 296 **ATOM** 1045 CA SER 296 76.118 39.695 24.521 1.00 33.38 ATOM 1046 CB SER 296 76.667 41.115 24.620 1.00 24.78 **ATOM** 1047 OG SER 77.368 41.478 23.449 1.00 25.43 296 ATOM 1048 C 296 SER 77.216 38.748 24.045 1.00 35.86 **ATOM** SER 296 1049 O 77.220 38.324 22.886 1.00 39.60 **ATOM** 1050 N ASP 297 78.135 38.402 24.943 1.00 37.41 1051 CA ASP **ATOM** 297 79.227 37.490 24.602 1.00 35.39 **ATOM** 1052 CB ASP 297 80.147 37.269 25.808 1.00 43.07 **ATOM** 1053 CG ASP 297 80.839 38.540 26.266 1.00 45.07 297 **ATOM** 1054 OD1 ASP 81.175 39.398 25.419 1.00 48.02 **ATOM** 1055 OD2 ASP 297 81.064 38.670 27.485 1.00 50.13 **ATOM** 1056 C ASP 297 78.662 36.145 24.161 1.00 30.87 **ATOM** 1057 O **ASP** 297 79.155 35.534 23.213 1.00 33.92 1058 N ALA 298 **ATOM** 77.625 35.698 24.861 1.00 28.96 **ATOM** 1059 CA ALA 298 76.971 34.428 24.574 1.00 30.60 **ATOM** 1060 CB ALA 298 75.889 34.157 25.610 1.00 27.56 **ATOM** 1061 C ALA 298 76.377 34.408 23.163 1.00 33.04 **ATOM** 1062 O ALA 298 76.538 33.426 22.426 1.00 32.48 **ATOM** 1063 N ILE 299 75.706 35.493 22.786 1.00 30.92 **ATOM** 1064 CA ILE 299 75.091 35.588 21.468 1.00 24.71 1065 CB ILE **ATOM** 299 74.138 36.789 21.368 1.00 22.98 **ATOM** 1066 CG2 ILE 299 73.430 36.786 20.018 1.00 21.90 299 73.091 36.707 22.477 1.00 20.91 **ATOM** 1067 CG1 ILE **ATOM** 1068 CD1 ILE 299 72.266 37.951 22.634 1.00 19.86 **ATOM** 1069 C ILE 299 76.168 35.680 20.395 1.00 26.77 **ATOM** 1070 O ILE 299 76.036 35.069 19.335 1.00 30.21 **ATOM** 1071 N PHE 300 77.238 36.428 20.673 1.00 29.08 78.345 36.562 19.726 1.00 28.06 **ATOM** 1072 CA PHE 300 300 **ATOM** 1073 CB PHE 79.386 37.565 20.235 1.00 29.06 **ATOM** 1074 CG PHE 300 79.289 38.920 19.590 1.00 28.14 **ATOM** 1075 CD1 PHE 300 78.449 39.896 20.113 1.00 27.20 1076 CD2 PHE 300 **ATOM** 80.017 39.209 18.437 1.00 29.11 **ATOM** 1077 CE1 PHE 300 78.332 41.139 19.499 1.00 28.18 1078 CE2 PHE 300 **ATOM** 79.908 40.450 17.815 1.00 29.07 1079 CZ PHE 300 ATOM 79.064 41.416 18.348 1.00 22.61 **ATOM** 1080 C PHE 300 78.991 35.201 19.485 1.00 29.00 PHE ATOM 1081 O 300 79.278 34.833 18.344 1.00 30.35 1082 N GLU 301 **ATOM** 79.183 34.442 20.560 1.00 31.81 **ATOM** 1083 CA GLU 301 79.767 33.111 20.470 1.00 34.96 1084 CB GLU **ATOM** 301 79.962 32.528 21.865 1.00 30.78 **ATOM** 1085 C GLU 301 78.850 32.210 19.634 1.00 35.49

ATOM 1086 O GLU 79.322 31.438 18.793 1.00 35.76 301 **ATOM** 1087 N LEU 302 77.543 32.313 19.869 1.00 32.14 **ATOM** 1088 CA LEU 302 76.559 31.522 19.132 1.00 25.56 **ATOM** 1089 CB LEU 302 75.147 31.760 19.682 1.00 23.33 1090 CG LEU **ATOM** 302 73.992 31.006 19.010 1.00 28.73 ATOM 1091 CD1 LEU 74.093 29.509 19.270 1.00 23.93 302 **ATOM** 1092 CD2 LEU 302 72.667 31.551 19.514 1.00 21.32 1093 C **ATOM** LEU 302 76.617 31.885 17.650 1.00 23.10 **ATOM** 1094 O LEU 302 76.664 31.001 16.796 1.00 26.79 **ATOM** 1095 N GLY 303 76.672 33.181 17.353 1.00 22.79 **ATOM** 1096 CA GLY 303 76.745 33.631 15.974 1.00 21.60 ATOM 1097 C GLY 303 77.978 33.104 15.256 1.00 30.42 ATOM 1098 O **GLY** 303 77.889 32.619 14.125 1.00 29.18 **ATOM** 1099 N **ALA** 304 79.132 33.182 15.912 1.00 31.15 **ATOM** 1100 CA ALA 304 80.375 32.703 15.313 1.00 35.44 **ATOM** 1101 CB ALA 304 81.562 32.995 16.235 1.00 29.16 **ATOM** 1102 C ALA 80.300 31.208 14.978 1.00 35.15 304 **ATOM** 1103 O ALA 304 80.705 30.785 13.891 1.00 37.13 **ATOM** 1104 N SER 305 79.753 30.414 15.892 1.00 33.91 **ATOM** 1105 CA SER 305 79.638 28.979 15.663 1.00 36.39 ATOM 1106 CB SER 305 79.395 28.237 16.980 1.00 32.71 **ATOM** 1107 OG SER 305 78.265 28.749 17.663 1.00 48.66 ATOM 1108 C SER 305 78.558 28.619 14.641 1.00 37.61 ATOM 1109 O SER 78.747 27.697 13.845 1.00 39.92 305 **ATOM** 1110 N LEU 306 77.443 29.349 14.651 1.00 38.21 **ATOM** 1111 CA LEU 306 76.350 29.092 13.714 1.00 35.65 **ATOM** 1112 CB LEU 306 75.094 29.894 14.077 1.00 25.49 ATOM 1113 CG LEU 306 74.209 29.374 15.212 1.00 26.18 ATOM 1114 CD1 LEU 306 72.988 30.262 15.361 1.00 23.40 **ATOM** 1115 CD2 LEU 306 73.777 27.952 14.921 1.00 23.57 **ATOM** 1116 C LEU 306 76.723 29.356 12.258 1.00 38.05 **ATOM** 1117 O LEU 306 76.092 28.809 11.353 1.00 37.22 **ATOM** 1118 N SER 307 77.743 30.185 12.030 1.00 40.41 ATOM 1119 CA SER 307 78.199 30.511 10.677 1.00 40.85 **ATOM** 1120 CB SER 307 79.415 31.442 10.736 1.00 37.32 ATOM 79.086 32.678 11.344 1.00 56.20 1121 OG SER 307 **ATOM** 1122 C SER 307 78.550 29.270 9.852 1.00 39.87 **ATOM** SER 1123 O 307 78.221 29.191 8.670 1.00 44.27 1124 N **ATOM** ALA 308 79.207 28.305 10.487 1.00 39.29 **ATOM** 1125 CA ALA 308 79.609 27.066 9.826 1.00 33.10 **ATOM** 1126 CB ALA 308 80.607 26.310 10.696 1.00 33.37 **ATOM** 1127 C ALA 308 78.403 26.177 9.502 1.00 34.07 **ATOM** 1128 O ALA 308 78.467 25.340 8.600 1.00 40.61 **ATOM** 1129 N PHE 309 77.305 26.368 10.230 1.00 31.85 ATOM 1130 CA PHE 309 76.095 25.581 10.015 1.00 35.24 **ATOM** 1131 CB PHE 309 75.149 25.698 11.219 1.00 33.69 **ATOM** 1132 CG PHE 309 75.618 24.954 12.437 1.00 36.16

ATOM	1133 CD1 PHE 309	76.785 25.327 13.090 1.00 43.79
ATOM		
ATOM	· ·	
ATOM		
ATOM		76.514 23.543 14.683 1.00 38.37
ATOM		75.361 25.934 8.720 1.00 36.31
ATOM		74.633 25.095 8.173 1.00 37.84
ATOM	1140 N ASN 310	75.567 27.155 8.225 1.00 35.22
ATOM	1141 CA ASN 310	74.933 27.625 6.988 1.00 43.66
ATOM	1142 CB ASN 310	75.536 26.930 5.760 1.00 54.13
ATOM	1143 CG ASN 310	76.980 27.339 5.501 1.00 68.29
ATOM	1144 OD1 ASN 310	77.297 28.527 5.412 1.00 74.62
ATOM	1145 ND2 ASN 310	77.859 26.348 5.352 1.00 68.85
ATOM	1146 C ASN 310	73.430 27.385 7.013 1.00 38.37
ATOM	1147 O ASN 310	72.882 26.735 6.123 1.00 36.70
ATOM	1148 N LEU 311	72.780 27.865 8.062 1.00 35.22
ATOM	1149 CA LEU 311	71.345 27.690 8.206 1.00 34.32
ATOM	1150 CB LEU 311	70.895 28.054 9.630 1.00 30.19
ATOM	1151 CG LEU 311	71.458 27.306 10.845 1.00 26.76
ATOM	1152 CD1 LEU 311	70.792 27.847 12.104 1.00 21.37
ATOM	1153 CD2 LEU 311	71.217 25.813 10.722 1.00 22.95
ATOM	1154 C LEU 311	70.601 28.561 7.206 1.00 34.64
ATOM	1155 O LEU 311	71.087 29.625 6.820 1.00 37.70
ATOM	1156 N ASP 312	69.444 28.091 6.752 1.00 29.40
ATOM ATOM	1157 CA ASP 312 1158 CB ASP 312	68.634 28.867 5.823 1.00 28.65
ATOM	1150 CB ASP 312	68.302 28.061 4.545 1.00 24.79 67.459 26.804 4.804 1.00 21.47
ATOM	1160 OD1 ASP 312	67.459 26.804 4.804 1.00 21.47 66.994 26.549 5.932 1.00 27.92
ATOM	1161 OD2 ASP 312	67.250 26.057 3.832 1.00 27.53
ATOM	1162 C ASP 312	67.380 29.346 6.557 1.00 25.92
ATOM	1163 O ASP 312	67.167 28.985 7.717 1.00 26.98
ATOM	1164 N ASP 313	66.540 30.122 5.878 1.00 21.78
ATOM	1165 CA ASP 313	65.315 30.653 6.471 1.00 22.89
ATOM	1166 CB ASP 313	64.517 31.458 5.439 1.00 29.19
ATOM	1167 CG ASP 313	65.216 32.739 5.025 1.00 36.82
ATOM	1168 OD1 ASP 313	65.985 33.285 5.845 1.00 41.51
ATOM	1169 OD2 ASP 313	64.997 33.203 3.883 1.00 44.19
ATOM	1170 C ASP 313	64.421 29.587 7.085 1.00 25.09
ATOM	1171 O ASP 313	63.778 29.829 8.110 1.00 27.60
ATOM	1172 N THR 314	64.363 28.420 6.449 1.00 20.90
ATOM	1173 CA THR 314	63.538 27.322 6.942 1.00 22.71
ATOM	1174 CB THR 314	63.408 26.208 5.884 1.00 22.07
ATOM	1175 OG1 THR 314	62.825 26.746 4.693 1.00 23.15
ATOM	1176 CG2 THR 314	62.542 25.079 6.401 1.00 18.17
ATOM	1177 C THR 314	64.080 26.734 8.249 1.00 19.95
ATOM	1178 O THR 314	63.326 26.477 9.182 1.00 22.40
ATOM	1179 N GLU 315	65.391 26.536 8.318 1.00 20.01

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ATOM	1180 CA GLU 315	65.997 25.987 9.523 1.00 19.40
ATOM	1181 CB GLU 315	67.454 25.626 9.254 1.00 11.72
ATOM	1182 CG GLU 315	67.544 24.440 8.322 1.00 13.43
ATOM	1183 CD GLU 315	68.925 24.157 7.791 1.00 18.51
ATOM	1184 OE1 GLU 315	69.666 25.107 7.451 1.00 23.24
ATOM	1185 OE2 GLU 315	69.254 22.962 7.673 1.00 24.23
ATOM	1186 C GLU 315	65.833 26.960 10.681 1.00 20.12
ATOM	1187 O GLU 315	65.425 26.570 11.777 1.00 20.53
ATOM	1188 N VAL 316	66.055 28.240 10.406 1.00 21.79
ATOM	1189 CA VAL 316	65.898 29.270 11.425 1.00 18.14
ATOM	1190 CB VAL 316	66.346 30.659 10.898 1.00 18.97
ATOM	1191 CG1 VAL 316	66.040 31.741 11.929 1.00 19.08
ATOM	1192 CG2 VAL 316	67.840 30.641 10.537 1.00 17.97
ATOM	1193 C VAL 316	64.430 29.332 11.880 1.00 22.54
ATOM	1194 O VAL 316	64.146 29.433 13.072 1.00 26.47
ATOM	1195 N ALA 317	63.505 29.242 10.924 1.00 19.66
ATOM	1196 CA ALA 317	62.076 29.286 11.216 1.00 16.99
ATOM	1197 CB ALA 317	61.279 29.329 9.926 1.00 17.79
ATOM	1198 C ALA 317	61.619 28.105 12.063 1.00 14.12
ATOM	1199 O ALA 317	60.808 28.263 12.970 1.00 17.04
ATOM	1200 N LEU 318	62.104 26.911 11.740 1.00 20.37
ATOM	1201 CA LEU 318	61.725 25.714 12.485 1.00 21.12
ATOM	1202 CB LEU 318	62.131 24.448 11.718 1.00 21.80
ATOM	1203 CG LEU 318	61.364 24.265 10.398 1.00 18.11
ATOM	1204 CD1 LEU 318	61.946 23.125 9.594 1.00 16.79
ATOM	1205 CD2 LEU 318 1206 C LEU 318	59.891 24.024 10.676 1.00 12.66
ATOM ATOM		62.335 25.752 13.880 1.00 22.03
ATOM	1207 O LEU 318 1208 N LEU 319	61.688 25.373 14.858 1.00 21.35 63.564 26.257 13.964 1.00 20.03
ATOM	1209 CA LEU 319	63.564 26.257 13.964 1.00 20.03 64.260 26.395 15.236 1.00 20.24
ATOM	1210 CB LEU 319	65.657 26.960 15.001 1.00 19.07
ATOM	1211 CG LEU 319	66.594 27.108 16.196 1.00 27.61
	1212 CD1 LEU 319	66.518 25.883 17.083 1.00 29.73
ATOM	1213 CD2 LEU 319	68.012 27.326 15.699 1.00 20.98
ATOM	1214 C LEU 319	63.422 27.334 16:118 1.00 21.16
ATOM	1215 O LEU 319	63.144 27.032 17.279 1.00 26.65
ATOM	1216 N GLN 320	62.958 28.439 15.539 1.00 20.77
ATOM	1217 CA GLN 320	62.119 29.390 16.265 1.00 17.87
ATOM	1218 CB GLN 320	61.781 30.594 15.388 1.00 18.74
ATOM	1219 CG GLN 320	62.957 31.496 15.111 1.00 21.07
ATOM	1220 CD GLN 320	62.637 32.617 14.150 1.00 22.88
ATOM	1221 OE1 GLN 320	61.571 32.653 13.528 1.00 26.07
ATOM	1222 NE2 GLN 320	63.574 33.537 14.006 1.00 20.11
ATOM	1223 C GLN 320	60.829 28.728 16.730 1.00 19.08
ATOM	1224 O GLN 320	60.368 28.976 17.844 1.00 23.39
ATOM	1225 N ALA 321	60.251 27.886 15.876 1.00 22.71
ATOM	1226 CA ALA 321	59.010 27.187 16.201 1.00 18.86

ATOM 1227 CB ALA 321 58.495 26.422 14.993 1.00 17.22 1228 C **ATOM ALA** 59.220 26.235 17.376 1.00 19.85 321 **ATOM** 1229 O ALA 321 58.362 26.119 18.250 1.00 19.60 **ATOM** 1230 N VAL 322 60.368 25.561 17.396 1.00 20.25 **ATOM** 1231 CA VAL 322 60.693 24.628 18.469 1.00 21.32 ATOM 1232 CB VAL 322 61.956 23.800 18.116 1.00 20.46 ATOM 1233 CG1 VAL 322 62.418 22.971 19.304 1.00 20.39 ATOM 1234 CG2 VAL 322 61.662 22.890 16.930 1.00 16.83 ATOM 1235 C VAL 322 60.880 25.393 19.785 1.00 20.67 **ATOM** 1236 O VAL 322 60.444 24.941 20.850 1.00 21.28 **ATOM** 1237 N LEU 323 61.492 26.574 19.701 1.00 21.14 **ATOM** 1238 CA LEU 323 61.722 27.417 20.869 1.00 22.94 **ATOM** 1239 CB LEU 323 62.610 28.608 20.511 1.00 16.12 **ATOM** 1240 CG LEU 323 64.051 28.291 20.115 1.00 22.28 **ATOM** 1241 CD1 LEU 323 64.719 29.532 19.528 1.00 14.87 **ATOM** 1242 CD2 LEU 323 64.816 27.750 21.320 1.00 21.55 **ATOM** 1243 C LEU 323 60.398 27.932 21.410 1.00 22.55 LEU ATOM 1244 O 323 60.185 27.986 22.615 1.00 25.21 1245 N LEU 324 **ATOM** 59.507 28.300 20.502 1.00 24.15 **ATOM** 1246 CA LEU 324 58.200 28.827 20.855 1.00 19.88 **ATOM** 1247 CB LEU 324 57.499 29.384 19.608 1.00 15.20 324 **ATOM** 1248 CG LEU 56.067 29.908 19.767 1.00 17.21 **ATOM** 1249 CD1 LEU 324 56.021 31.161 20.637 1.00 15.99 ATOM 1250 CD2 LEU 324 55.496 30.208 18.395 1.00 20.03 **ATOM** 1251 C LEU 324 57.311 27.795 21.536 1.00 19.83 ATOM 1252 O LEU 324 56.767 28.064 22.609 1.00 24.47 1253 N **MET** 325 **ATOM** 57.197 26.603 20.956 1.00 25.02 **ATOM** 1254 CA MET 325 56.339 25.563 21.522 1.00 26.72 **ATOM** 1255 CB MET 325 55.823 24.644 20.410 1.00 30.03 1256 CG MET **ATOM** 325 55.129 25.358 19.241 1.00 25.09 **ATOM** 1257 SD MET 325 53.714 26.409 19.672 1.00 27.29 **ATOM** 1258 CE MET 325 52.503 25.220 20.084 1.00 20.67 ATOM 1259 C **MET** 325 56.995 24.736 22.635 1.00 28.94 **ATOM** 1260 O **MET** 325 56.881 23.510 22.672 1.00 32.94 **ATOM** 1261 N SER 326 57.642 25.418 23.569 1.00 29.36 **ATOM** 1262 CA SER 326 58.311 24.759 24.680 1.00 31.62 1263 CB SER **ATOM** 326 59.554 25.559 25.064 1.00 38.13 **ATOM** 1264 OG SER 326 60.277 24.949 26.119 1.00 48.99 57.361 24.653 25.871 1.00 33.69 **ATOM** 1265 C SER 326 1266 O SER 326 **ATOM** 56.620 25.594 26.166 1.00 33.66 **ATOM** 1267 N THR 327 57.356 23.499 26.536 1.00 38.27 **ATOM** 1268 CA THR 327 56.497 23.306 27.701 1.00 38.98 1269 CB THR **ATOM** 327 55.875 21.896 27.730 1.00 33.30 56.908 20.911 27.627 1.00 44.01 **ATOM** 1270 OG1 THR 327 1271 CG2 THR 327 **ATOM** 54.888 21.722 26.587 1.00 38.09 **ATOM** 1272 C THR 327 57.239 23.570 29.018 1.00 42.88 **ATOM** 1273 O THR 327 56.702 23.325 30.099 1.00 43.36

ATOM 1274 N ASP 328 58.462 24.091 28.924 1.00 45.92 **ATOM** 1275 CA ASP 328 59.268 24.410 30.104 1.00 49.59 **ATOM** 1276 CB ASP 328 60.760 24.411 29.760 1.00 59.87 **ATOM** 1277 CG ASP 328 61.273 23.040 29.387 1.00 75.73 **ATOM** 1278 OD1 ASP 328 62.008 22.939 28.382 1.00 85.81 **ATOM** 1279 OD2 ASP 328 60.946 22.063 30.098 1.00 85.56 **ATOM** 1280 C **ASP** 328 58.873 25.767 30.673 1.00 48.50 328 **ATOM** 1281 O **ASP** 59.725 26.609 30.961 1.00 57.50 **ARG ATOM** 1282 N 329 57.569 25.980 30.805 1.00 49.62 **ATOM** 1283 CA ARG 329 57.032 27.222 31.340 1.00 50.52 **ATOM** 1284 CB ARG 329 56.400 28.080 30.230 1.00 53.57 **ATOM** 1285 CG ARG 57.376 28.828 29.324 1.00 51.09 329 **ATOM** 1286 CD ARG 329 57.897 27.951 28.204 1.00 49.73 **ATOM** 1287 NE ARG 329 58.692 28.699 27.233 1.00 47.44 **ATOM** 1288 CZ ARG 329 60.005 28.569 27.080 1.00 54.28 **ATOM** 1289 NH1 ARG 329 60.688 27.722 27.839 1.00 58.35 **ATOM** 1290 NH2 ARG 329 60.631 29.256 26.136 1.00 51.92 **ATOM** 1291 C ARG 329 55.970 26.870 32.375 1.00 51.90 **ATOM** 1292 O ARG 329 55.378 25.790 32.324 1.00 50.77 **ATOM** 1293 N SER 330 55.728 27.784 33.303 1.00 50.56 **ATOM** 1294 CA SER 330 54.744 27.564 34.349 1.00 50.67 **ATOM** 1295 CB SER 330 55.271 28.108 35.678 1.00 46.64 **ATOM** 1296 C SER 330 53.404 28.213 34.004 1.00 47.63 **ATOM** 1297 O SER 330 53.371 29.309 33.440 1.00 48.02 **ATOM** 1298 N GLY 331 52.314 27.496 34.277 1.00 44.44 **ATOM** 1299 CA GLY 331 50.977 28.023 34.044 1.00 38.77 **ATOM** 1300 C GLY 331 50.236 27.710 32.756 1.00 41.74 **ATOM** 1301 O **GLY** 331 49.147 28.246 32.537 1.00 49.57 **ATOM** 1302 N LEU 332 50.783 26.841 31.912 1.00 39.75 **ATOM** 1303 CA LEU 332 50.123 26.502 30.651 1.00 37.55 **ATOM** 1304 CB LEU 332 51.107 25.829 29.694 1.00 32.36 **ATOM** 1305 CG LEU 332 52.268 26.659 29.153 1.00 34.40 1306 CD1 LEU **ATOM** 332 53.207 25.749 28.379 1.00 30.22 **ATOM** 1307 CD2 LEU 332 51.742 27.786 28.277 1.00 23.33 1308 C LEU **ATOM** 332 48.921 25.589 30.834 1.00 36.73 **ATOM** 1309 O LEU 332 48.987 24.608 31.577 1.00 39.29 **ATOM** 1310 N LEU 333 47.822 25.925 30.168 1.00 36.07 **ATOM** 1311 CA LEU 333 46.615 25.107 30.215 1.00 39.58 ATOM 1312 CB LEU 333 45.384 25.906 29.754 1.00 41.08 **ATOM** 1313 CG LEU 333 44.601 26.883 30.644 1.00 47.59 **ATOM** 1314 CD1 LEU 333 44.268 26.213 31.961 1.00 45.65 **ATOM** 1315 CD2 LEU 333 45.366 28.171 30.874 1.00 47.42 **ATOM** 1316 C LEU 333 46.791 23.911 29.278 1.00 40.00 **ATOM** 1317 O LEU 333 46.690 22.754 29.689 1.00 44.77 **ATOM** 1318 N CYA 334 47.102 24.213 28.022 1.00 37.70 **ATOM** 1319 CA CYA 334 47.265 23.209 26.968 1.00 36.04 **ATOM** 1320 CB CYA 334 46.815 23.808 25.635 1.00 40.64

1321 SG CYA 334 **ATOM** 45.280 24.738 25.758 1.00 44.31 ATOM 1322 AS CYA 334 43.972 22.946 25.380 1.00 76.30 **ATOM** 1323 C CYA 334 48.668 22.617 26.815 1.00 34.91 **ATOM** 1324 O **CYA** 334 49.237 22.615 25.722 1.00 37.63 **ATOM** 1325 N VAL 335 49.189 22.056 27.903 1.00 35.43 **ATOM** 1326 CA VAL 335 50.518 21.452 27.909 1.00 34.27 **ATOM** 1327 CB VAL 335 50.861 20.868 29.298 1.00 34.21 ATOM 1328 CG1 VAL 335 52.261 20.258 29.292 1.00 33.66 ATOM 1329 CG2 VAL 335 50.755 21.945 30.362 1.00 31.77 **ATOM** 1330 C VAL 335 50.662 20.349 26.865 1.00 37.14 **ATOM** 1331 O VAL 335 51.639 20.320 26.114 1.00 37.59 **ATOM** 1332 N **ASP** 336 49.683 19.451 26.813 1.00 39.99 1333 CA ASP ATOM 336 49.705 18.339 25.866 1.00 41.64 **ATOM** 1334 CB ASP 336 48.532 17.392 26.146 1.00 54.27 ATOM 1335 CG ASP 336 48.596 16.118 25.322 1.00 67.42 **ATOM** 1336 OD1 ASP 336 47.915 16.049 24.274 1.00 70.98 **ATOM** 1337 OD2 ASP 336 49.337 15.191 25.717 1.00 76.88 **ATOM** 1338 C **ASP** 336 49.702 18.762 24.393 1.00 38.31 ATOM 1339 O **ASP** 336 50.469 18.229 23.586 1.00 37.46 ATOM 1340 N LYS 337 48.853 19.729 24.052 1.00 30.23 **ATOM** 1341 CA LYS 337 48.740 20.211 22.676 1.00 29.21 **ATOM** 1342 CB LYS 337 47.561 21.189 22.559 1.00 30.53 ATOM 1343 CG LYS 337 47.012 21.360 21.162 1.00 51.63 **ATOM** 1344 CD LYS 337 45.636 21.997 21.186 1.00 59.57 **ATOM** 1345 CE LYS 337 45.066 22.115 19.774 1.00 66.05 337 **ATOM** 1346 NZ LYS 43.673 22.693 19.776 1.00 67.20 **ATOM** 1347 C LYS 337 50.054 20.873 22.249 1.00 28.33 **ATOM** 1348 O LYS 337 50.581 20.594 21.170 1.00 26.08 **ATOM** 1349 N ILE 338 50.609 21.696 23.141 1.00 26.74 ATOM . 1350 CA ILE 338 51.873 22.390 22.902 1.00 25.42 **ATOM** 1351 CB ILE 338 52.177 23.379 24.052 1.00 23.57 **ATOM** 1352 CG2 ILE 338 53.559 23.991 23.874 1.00 22.59 **ATOM** 1353 CG1 ILE 338 51.105 24.471 24.096 1.00 23.57 **ATOM** 1354 CD1 ILE 338 51.157 25.362 25.333 1.00 24.30 **ATOM** 1355 C ILE 338 53.018 21.382 22.768 1.00 29.20 **ATOM** 1356 O ILE 338 53.905 21.537 21.916 1.00 31.59 **ATOM** 1357 N **GLU** 339 52.977 20.340 23.595 1.00 34.82 1358 CA GLU 339 **ATOM** 53.980 19.277 23.597 1.00 34.23 339 **ATOM** 1359 CB GLU 53.639 18.256 24.681 1.00 40.38 **ATOM** 1360 CG GLU 339 54.785 17.354 25.072 1.00 54.98 339 ATOM 1361 CD GLU 55.644 17.964 26.178 1.00 71.26 **ATOM** 339 1362 OE1 GLU 56.766 18.444 25.858 1.00 77.82 **ATOM** 1363 OE2 GLU 339 55.170 17.985 27.349 1.00 65.14 **ATOM** 1364 C **GLU** 339 53.972 18.582 22.231 1.00 34.42 **ATOM** 1365 O **GLU** 339 55.018 18.431 21.590 1.00 29.41 **ATOM** 1366 N LYS 340 52.778 18.189 21.786 1.00 34.13 **ATOM** 1367 CA LYS 340 52.592 17.513 20.502 1.00 32.05

ATOM 1368 CB LYS 340 51.121 17.105 20.3 ATOM 1369 C LYS 340 53.064 18.390 19.3 ATOM 1370 O LYS 340 53.762 17.913 18.4 ATOM 1371 N SER 341 52.725 19.677 19.3	37 1.00 32.56 41 1.00 32.93 74 1.00 31.42 34 1.00 27.79 01 1.00 27.85
ATOM 1370 O LYS 340 53.762 17.913 18.4 ATOM 1371 N SER 341 52.725 19.677 19.3	41 1.00 32.93 74 1.00 31.42 34 1.00 27.79 01 1.00 27.85
ATOM 1371 N SER 341 52.725 19.677 19.3	74 1.00 31.42 34 1.00 27.79 01 1.00 27.85
17.0	34 1.00 27.79 01 1.00 27.85
	01 1.00 27.85
ATOM 1372 CA SER 341 53.134 20.621 18.3	
ATOM 1373 CB SER 341 52.559 22.009 18.6	70 1 00 47 00
ATOM 1374 OG SER 341 51.149 21.966 18.5	
ATOM 1375 C SER 341 54.647 20.713 18.24	
ATOM 1376 O SER 341 55.205 20.706 17.13	
ATOM 1377 N GLN 342 55.318 20.794 19.3	— -
ATOM 1378 CA GLN 342 56.771 20.875 19.3	
ATOM 1379 CB GLN 342 57.309 21.089 20.7	· · -
ATOM 1380 CG GLN 342 58.768 21.466 20.7	
ATOM 1381 CD GLN 342 59.407 21.429 22.1 ATOM 1382 OE1 GLN 342 60.123 22.356 22.5	
ATOM 1383 NE2 GLN 342 59.184 20.345 22.8 ATOM 1384 C GLN 342 57.377 19.609 18.78	
ATOM 1385 O GLN 342 58.378 19.675 18.06	· · · · · -
ATOM 1386 N GLU 343 56.777 18.458 19.07	
ATOM 1387 CA GLU 343 57.251 17.190 18.5	
ATOM 1388 CB GLU 343 56.462 16.016 19.1	
ATOM 1389 CG GLU 343 56.812 15.700 20.5	
ATOM 1390 CD GLU 343 55.951 14.594 21.1	
ATOM 1391 OE1 GLU 343 55.472 13.719 20.4	=
ATOM 1392 OE2 GLU 343 55.758 14.601 22.4	
ATOM 1393 C GLU 343 57.097 17.225 17.00	
ATOM 1394 O GLU 343 58.008 16.842 16.26	0 1.00 27.26
ATOM 1395 N ALA 344 55.947 17.727 16.55	0 1.00 23.70
ATOM 1396 CA ALA 344 55.647 17.853 15.13	24 1.00 22.16
ATOM 1397 CB ALA 344 54.275 18.489 14.92	27 1.00 21.18
ATOM 1398 C ALA 344 56.729 18.694 14.45	
ATOM 1399 O ALA 344 57.303 18.284 13.43	
ATOM 1400 N TYR 345 57.048 19.840 15.05	
ATOM 1401 CA TYR 345 58.073 20.738 14.53	
ATOM 1402 CB TYR 345 58.085 22.059 15.30	
ATOM 1403 CG TYR 345 57.023 23.015 14.83 ATOM 1404 CD1 TYR 345 56.004 23.434 15.60	
ATOM 1406 CD2 TYR 345 57.003 23.448 13.50 ATOM 1407 CE2 TYR 345 55.991 24.269 13.03	
ATOM 1407 CEZ TTR 345 53.991 24.209 13.03 ATOM 1408 CZ TYR 345 54.984 24.668 13.89	
ATOM 1408 CZ 11R 343 54,364 24,008 13,89 ATOM 1409 OH TYR 345 53,963 25,455 13,40	
ATOM 1409 OH 11R 343 35.903 25.433 15.40 ATOM 1410 C TYR 345 59.465 20.120 14.548	
ATOM 1411 O TYR 345 60.238 20.291 13.593	
ATOM 1412 N LEU 346 59.777 19.401 15.621	
ATOM 1413 CA LEU 346 61.074 18.746 15.76	
ATOM 1414 CB LEU 346 61.207 18.108 17.15	

ATOM 1415 CG LEU 346 61.637 19.076 18.252 1.00 26.46 **ATOM** 1416 CD1 LEU 346 61.387 18.468 19.610 1.00 26.46 **ATOM** 1417 CD2 LEU 346 63.101 19.437 18.076 1.00 21.78 **ATOM** 1418 C LEU 346 61.322 17.713 14.683 1.00 23.24 **ATOM** 1419 O LEU 346 62.416 17.645 14.127 1.00 27.54 1420 N LEU ATOM 60.314 16.900 14.395 1.00 25.75 347 1421 CA LEU **ATOM** 347 60.437 15.881 13.356 1.00 25.41 **ATOM** 1422 CB LEU 347 59.208 14.970 13.330 1.00 23.78 **ATOM** 1423 CG LEU 347 59.302 13.713 14.190 1.00 31.85 ATOM 1424 CD1 LEU 347 58.004 12.928 14.089 1.00 39.88 **ATOM** 1425 CD2 LEU 347 60.483 12.864 13.738 1.00 27.65 **ATOM** 1426 C LEU 347 60.611 16.535 11.998 1.00 23.22 ATOM 1427 O LEU 347 61.468 16.133 11.211 1.00 28.58 1428 N **ATOM** ALA 348 59.784 17.542 11.731 1.00 26.40 **ATOM** 1429 CA ALA 348 59.840 18.273 10.474 1.00 23.85 **ATOM** 1430 CB ALA 348 58.732 19.324 10.433 1.00 25.27 **ATOM** 1431 C ALA 348 61.210 18.924 10.337 1.00 23.69 1432 O ALA **ATOM** 348 61.847 18.835 9.288 1.00 29.11 1433 N PHE 349 **ATOM** 61.678 19.506 11.438 1.00 24.71 **ATOM** 1434 CA PHE 349 62.973 20.181 11.493 1.00 20.48 1435 CB PHE 349 **ATOM** 63.164 20.772 12.900 1.00 17.84 1436 CG PHE 349 **ATOM** 64.334 21.721 13.031 1.00 14.90 ATOM 1437 CD1 PHE 349 65.109 22.069 11.933 1.00 17.58 ATOM 1438 CD2 PHE 349 64.651 22.269 14.271 1.00 24.77 **ATOM** 1439 CE1 PHE 349 66.185 22.944 12.063 1.00 20.26 **ATOM** 1440 CE2 PHE 349 65.727 23.147 14.413 1.00 23.83 **ATOM** 1441 CZ PHE 349 66.494 23.486 13.299 1.00 20.36 **ATOM** 1442 C PHE 349 64.084 19.181 11.159 1.00 23.43 349 **ATOM** 1443 O PHE 64.916 19.427 10.278 1.00 24.35 **ATOM** 1444 N GLU 350 64.057 18.028 11.820 1.00 25.79 **ATOM** 1445 CA GLU 350 65.060 16.991 11.606 1.00 26.75 ATOM, 1446 CB GLU 350 64.813 15.822 12.567 1.00 29.56 ATOM 1447 CG GLU 350 65.774 14.661 12.391 1.00 39.94 **ATOM** 1448 CD GLU 350 65.574 13.549 13.407 1.00 45.06 **ATOM** 1449 OE1 GLU 350 64.413 13.192 13.715 1.00 49.26 **ATOM** 1450 OE2 GLU 350 66.593 13.017 13.887 1.00 56.67 1451 C GLU **ATOM** 350 65.051 16.494 10.162 1.00 26.95 **ATOM** 1452 O GLU 350 66.096 16.398 9.513 1.00 28.77 **ATOM** 1453 N HIS 351 63.858 16.219 9.652 1.00 22.56 1454 CA HIS ATOM 351 63.699 15.728 8.294 1.00 22.20 **ATOM** 1455 CB HIS 351 62.263 15.265 8.083 1.00 22.47 **ATOM** 1456 CG HIS 351 61.881 14.106 8.947 1.00 23.61 1457 CD2 HIS 351 **ATOM** 62.633 13.300 9.739 1.00 27.65 ATOM 1458 ND1 HIS 351 60.585 13.653 9.069 1.00 26.13 351 **ATOM** 1459 CE1 HIS 60.548 12.629 9.898 1.00 22.87 **ATOM** 1460 NE2 HIS 351 61.779 12.393 10.319 1.00 27.53 ATOM 1461 C HIS 351 64.135 16.764 7.259 1.00 21.76

ATOM 1462 O HIS 351 64.708 16.419 6.226 1.00 27.02 1463 N **ATOM** TYR 352 63.909 18.041 7.555 1.00 18.26 **ATOM** 1464 CA TYR 352 64.327 19.101 6.649 1.00 16.94 **ATOM** 1465 CB TYR 352 63.749 20.455 7.066 1.00 19.07 **ATOM** 1466 CG TYR 352 64.107 21.534 6.081 1.00 21.11 ATOM 1467 CD1 TYR 352 63.518 21.564 4.819 1.00 21.33 352 ATOM 1468 CE1 TYR 63.921 22.482 3.859 1.00 21.06 **ATOM** 1469 CD2 TYR 352 65.105 22.462 6.367 1.00 22.07 **ATOM** 1470 CE2 TYR 352 65.515 23.388 5.412 1.00 25.40 **ATOM** 1471 CZ TYR 352 64.921 23.384 4.161 1.00 21.90 1472 OH TYR 352 **ATOM** 65.334 24.268 3.197 1.00 23.57 **ATOM** 1473 C **TYR** 352 65.853 19.156 6.657 1.00 18.49 **ATOM** 1474 O TYR 352 66.487 19.323 5.609 1.00 24.99 **ATOM** 1475 N VAL 353 66.451 19.008 7.836 1.00 24.64 1476 CA VAL **ATOM** 353 67.904 19.011 7.955 1.00 22.20 ATOM 1477 CB VAL 353 68.350 18.925 9.440 1.00 23.72 ATOM 1478 CG1 VAL 353 69.838 18.597 9.546 1.00 21.24 **ATOM** 1479 CG2 VAL 353 68.063 20.245 10.142 1.00 20.07 **ATOM** 1480 C VAL 353 68.452 17.829 7.146 1.00 25.07 ATOM 1481 O VAL 353 69.467 17.955 6.457 1.00 24.75 **ASN ATOM** 1482 N 354 67.768 16.690 7.221 1.00 24.59 1483 CA ASN **ATOM** 354 68.171 15.502 6.474 1.00 25.64 **ATOM** 1484 CB ASN 354 67.223 14.331 6.751 1.00 26.05 ATOM: 1485 CG ASN 354 67.368 13.763 8.151 1.00 30.27 **ATOM** 1486 OD1 ASN 354 66.443 13.139 8.672 1.00 33.71 **ATOM** 1487 ND2 ASN 354 68.529 13.959 8.765 1.00 34.78 **ATOM** 1488 C ASN 354 68.143 15.813 4.981 1.00 30.50 1489 O **ASN ATOM** 354 69.042 15.423 4.233 1.00 33.73 **ATOM** 1490 N HIS 355 67.098 16.519 4.555 1.00 30.54 **ATOM** 1491 CA HIS 355 66.926 16.901 3.157 1.00 26.02 **ATOM** 1492 CB HIS 355 65.535 17.521 2.953 1.00 29.93 **ATOM** 1493 CG HIS 355 65.367 18.217 1.638 1.00 37.91 **ATOM** 1494 CD2 HIS 355 65.654 19.486 1.264 1.00 31.26 **ATOM** 1495 ND1 HIS 355 64.861 17.593 0.518 1.00 32.67 **ATOM** 1496 CE1 HIS 355 64.843 18.447 -0.488 1.00 33.22 1497 NE2 HIS 355 **ATOM** 65.322 19.601 -0.061 1.00 32.69 **ATOM** 1498 C HIS 355 68.009 17.851 2.652 1.00 24.29 355 **ATOM** 1499 O HIS 68.381 17.798 1.484 1.00 26.82 **ATOM** 1500 N **ARG** 356 68.484 18.735 3.526 1.00 29.72 1501 CA ARG 356 **ATOM** 69.516 19.711 3.167 1.00 26.65 **ATOM** 1502 CB ARG 356 69.593 20.804 4.225 1.00 22.74 **ATOM** 1503 CG ARG 356 68.409 21.735 4.222 1.00 21.64 **ATOM** 1504 CD ARG 356 68.757 23.024 3.524 1.00 28.04 1505 NE ARG 356 **ATOM** 69.550 23.900 4.380 1.00 33.79 1506 CZ ARG 356 **ATOM** 70.508 24.716 3.952 1.00 29.26 **ATOM** 1507 NH1 ARG 356 70.814 24.776 2.667 1.00 29.08 71.136 25.493 4.816 1.00 33.61 ATOM 1508 NH2 ARG 356

ATOM 1509 C **ARG** 356 70.904 19.115 2.950 1.00 27.58 **ATOM** 1510 O **ARG** 356 71.757 19.740 2.312 1.00 31.44 1511 N **ATOM** LYS 357 71.140 17.937 3.519 1.00 30.56 **ATOM** 1512 CA LYS 357 72.422 17.244 3.390 1.00 34.56 **ATOM** 1513 CB LYS 357 72.500 16.518 2.043 1.00 39.66 **ATOM** 1514 CG LYS 357 71.476 15.402 1.871 1.00 42.16 **ATOM** 1515 CD LYS 357 71.674 14.676 0.550 1.00 54.23 **ATOM** 1516 CE LYS 357 70.691 13.523 0.371 1.00 61.97 **ATOM** 1517 NZ LYS 357 69.288 13.974 0.162 1.00 65.88 **ATOM** 1518 C LYS 357 73.665 18.119 3.606 1.00 36.73 **ATOM** 1519 O LYS 357 74.522 18.248 2.728 1.00 40.70 **ATOM** 1520 N HIS 358 73.738 18.732 4.786 1.00 33.69 **ATOM** 1521 CA HIS 358 74.863 19.581 5.163 1.00 33.59 **ATOM** 1522 CB HIS 358 74.660 20.155 6.571 1.00 32.07 **ATOM** 1523 CG HIS 358 73.593 21.200 6.666 1.00 29.74 **ATOM** 1524 CD2 HIS 358 72.245 21.098 6.736 1.00 23.35 **ATOM** 1525 ND1 HIS 358 73.876 22.547 6.731 1.00 28.13 **ATOM** 1526 CE1 HIS 358 72.752 23.231 6.834 1.00 26.94 **ATOM** 1527 NE2 HIS 358 71.747 22.373 6.838 1.00 23.32 **ATOM** 1528 C HIS 358 76.121 18.720 5.180 1.00 37.98 **ATOM** 1529 O HIS 358 76.087 17.581 5.654 1.00 41.07 ATOM 1530 N **ASN** 359 77.231 19.261 4.690 1.00 44.20 **ATOM** 1531 CA ASN 359 78.492 18.523 4.676 1.00 49.72 **ATOM** 1532 CB ASN 359 79.406 19.053 3.572 1.00 46.66 **ATOM ASN** 1533 C 359 79.174 18.648 6.039 1.00 51.77 **ATOM** 1534 O **ASN** 359 80.356 18.985 6.122 1.00 57.32 **ATOM** 1535 N ILE 360 78.414 18.383 7.101 1.00 51.04 1536 CA ILE **ATOM** 360 78.906 18.471 8.477 1.00 48.24 **ATOM** 1537 CB ILE 360 78.340 19.721 9.207 1.00 47.20 ATOM 1538 CG2 ILE 360 78.781 19.741 10.673 1.00 43.50 **ATOM** 1539 CG1 ILE 360 78.777 21.005 8.491 1.00 45.94 **ATOM** 1540 CD1 ILE 360 78.157 22.262 9.050 1.00 43.00 **ATOM** ILE 1541 C 360 78.462 17.222 9.239 1.00 47.23 **ATOM** 1542 O ILE 360 77.272 16.901 9.278 1.00 45.13 **ATOM** 1543 N PRO 361 79.416 16.490 9:838 1.00 48.61 **ATOM** 1544 CD PRO 361 80.869 16.705 9.729 1.00 50.93 **ATOM** 1545 CA PRO 361 79.129 15.270 10.599 1.00 45.46 80.524 14.725 10.927 1.00 49.01 **ATOM** 1546 CB PRO 361 **ATOM** 1547 CG PRO 361 81.402 15.307 9.862 1.00 54.41 **ATOM** 1548 C PRO 361 78.330 15.514 11.879 1.00 36.54 PRO **ATOM** 1549 O 361 78.666 16.394 12.672 1.00 39.83 1550 N HIS **ATOM** 362 77.282 14.716 12.075 1.00 31.35 **ATOM** 1551 CA HIS 362 76.430 14.798 13.264 1.00 33.34 **ATOM** 1552 CB HIS 362 77.246 14.495 14.524 1.00 33.77 **ATOM** 1553 CG HIS 362 78.129 13.292 14.397 1.00 34.40 **ATOM** 1554 CD2 HIS 362 77.837 11.999 14.130 1.00 32.60 79.501 13.362 14.506 1.00 36.14 **ATOM** 1555 ND1 HIS 362

ATOM 1556 CE1 HIS 362 80.017 12.160 14.311 1.00 36.26 1557 NE2 HIS **ATOM** 362 79.029 11.316 14.080 1.00 35.73 **ATOM** 1558 C HIS 362 75.778 16.164 13.389 1.00 33.55 **ATOM** 1559 O HIS 362 75.539 16.652 14.495 1.00 31.93 **ATOM** 1560 N PHE 363 75.449 16.748 12.240 1.00 35.83 ATOM 1561 CA PHE 363 74.834 18.067 12.166 1.00 30.93 **ATOM** 1562 CB PHE 363 74.464 18.394 10.712 1.00 28.82 **ATOM** 1563 CG PHE 363 73.959 19.797 10.514 1.00 26.59 **ATOM** 1564 CD1 PHE 363 74.846 20.843 10.301 1.00 26.96 **ATOM** 1565 CD2 PHE 363 72.596 20.076 10.575 1.00 27.51 **ATOM** 1566 CE1 PHE 363 74.384 22.151 10.155 1.00 31.83 **ATOM** 1567 CE2 PHE 363 72.124 21.378 10.433 1.00 26.65 ATOM 1568 CZ PHE 363 73.019 22.417 10.223 1.00 24.42 **ATOM** PHE 1569 C 363 73.613 18.235 13.063 1.00 28.73 **ATOM** 1570 O PHE 363 73.550 19.174 13.848 1.00 25.33 **ATOM** 1571 N TRP 364 72.663 17.310 12.969 1.00 22.89 **ATOM** 1572 CA TRP 364 71.443 17.405 13.760 1.00 24.19 **ATOM** 1573 CB TRP 364 70.481 16.254 13.439 1.00 26.31 **ATOM** 1574 CG TRP 364 69.198 16.275 14.228 1.00 20.24 ATOM 1575 CD2 TRP 364 68.213 17.325 14.262 1.00 24.50 1576 CE2 TRP **ATOM** 364 67.175 16.894 15.120 1.00 25.84 **ATOM** 1577 CE3 TRP 364 68.106 18.583 13.652 1.00 25.83 **ATOM** 1578 CD1 TRP 364 68.731 15.289 15.040 1.00 23.61 **ATOM** 1579 NE1 TRP 364 67.515 15.648 15.579 1.00 32.26 **ATOM** 1580 CZ2 TRP 364 66.048 17.674 15.386 1.00 21.95 **ATOM** 1581 CZ3 TRP 364 66.979 19.360 13.919 1.00 20.73 **ATOM** 1582 CH2 TRP 364 65.967 18.899 14.779 1.00 22.37 ATOM 1583 C TRP 364 71.663 17.551 15.267 1.00 28.84 **ATOM** 1584 O TRP 364 71.246 18.554 15.839 1.00 31.25 ATOM 1585 N PRO 365 72.305 16.568 15.932 1.00 29.69 **ATOM** 1586 CD PRO 365 72.790 15.245 15.497 1.00 30.89 **ATOM** 1587 CA PRO 365 72.499 16.748 17.373 1.00 25.62 **ATOM** 1588 CB PRO 365 73.195 15.451 17.810 1.00 25.50 **ATOM** 1589 CG PRO 365 73.804 14.915 16.560 1.00 34.15 **ATOM** 1590 C PRO 365 73.320 18.002 17.698 1.00 24.07 **ATOM** 1591 O PRO 365 73.079 18.654 18.711 1.00 23.58 **ATOM** 1592 N LYS 366 74.250 18.365 16.820 1.00 24.09 **ATOM** 1593 CA LYS 366 75.063 19.562 17.027 1.00 29.44 **ATOM** 1594 CB LYS 366 76.131 19.681 15.945 1.00 27.18 **ATOM** 1595 CG LYS 366 77.341 18.802 16.149 1.00 23.71 **ATOM** 1596 CD LYS 366 78.304 19.019 15.001 1.00 27.50 **ATOM** 1597 CE LYS 366 79.624 18.329 15.231 1.00 35.88 **ATOM** 1598 NZ LYS 366 80.550 18.591 14.097 1.00 41.92 **ATOM** 1599 C LYS 366 74.195 20.820 17.012 1.00 32.76 **ATOM** 1600 O LYS 366 74.326 21.694 17.873 1.00 36.13 **ATOM** 73.307 20.907 16.028 1.00 33.70 1601 N LEU 367 72.409 22.041 15.905 1.00 30.60 **ATOM** 1602 CA LEU 367

1603 CB LEU **ATOM** 367 71.636 21.955 14.587 1.00 24.26 **ATOM** 1604 CG LEU 367 70.675 23.103 14.274 1.00 32.42 **ATOM** 1605 CD1 LEU 367 71.394 24.440 14.404 1.00 24.78 **ATOM** 1606 CD2 LEU 70.098 22.924 12.878 1.00 28.84 367 **ATOM** 1607 C LEU 367 71.450 22.015 17.087 1.00 31.90 **ATOM** 1608 O LEU 367 71.113 23.052 17.655 1.00 39.20 **ATOM** 1609 N LEU 71.051 20.812 17.485 1.00 33.86 368 **ATOM** 1610 CA LEU 368 70.144 20.617 18.608 1.00 32.97 **ATOM** 1611 CB LEU 368 69.866 19.123 18.759 1.00 34.22 **ATOM** 1612 CG LEU 368 68.458 18.633 19.084 1.00 38.15 **ATOM** 1613 CD1 LEU 368 67.400 19.449 18.345 1.00 27.75 **ATOM** 1614 CD2 LEU 368 68.374 17.154 18.733 1.00 31.51 **ATOM** 1615 C LEU 368 70.793 21.181 19.875 1.00 35.29 **ATOM** 1616 O LEU 368 70.128 21.806 20.703 1.00 36.16 72.106 21.001 19.994 1.00 41.13 **ATOM** 1617 N MET 369 **ATOM** 1618 CA MET 369 72.857 21.504 21.139 1.00 40.92 **ATOM** 1619 CB MET 369 74.283 20.955 21.115 1.00 43.32 **ATOM** 1620 CG MET 369 74.383 19.497 21.545 1.00 50.01 **ATOM** 1621 SD MET 369 75.997 18.770 21.190 1.00 56.63 **ATOM** 1622 CE MET 369 77.032 19.596 22.409 1.00 62.26 **ATOM** 1623 C **MET** 369 72.872 23.032 21.186 1.00 43.46 1624 O ATOM **MET** 369 73.137 23.619 22.233 1.00 47.51 **ATOM** 1625 N LYS 370 72.594 23.673 20.053 1.00 41.60 **ATOM** 1626 CA LYS 370 72.561 25.131 19.988 1.00 34.48 **ATOM** 1627 CB LYS 370 72.689 25.623 18.546 1.00 31.53 **ATOM** 1628 CG LYS 370 74.012 25.278 17.896 1.00 30.76 **ATOM** 1629 CD LYS 370 75.168 25.774 18.731 1.00 32.16 1630 CE LYS 370 **ATOM** 76.488 25.388 18.116 1.00 31.08 **ATOM** 1631 NZ LYS 370 77.604 25.822 18.993 1.00 51.52 ATOM 1632 C LYS 370 71.269 25.652 20.606 1.00 36.35 LYS **ATOM** 1633 O 370 71.197 26.806 21.032 1.00 39.02 **ATOM** 1634 N VAL 371 70.248 24.804 20.652 1.00 34.33 **ATOM** 1635 CA VAL 371 68.975 25.186 21.249 1.00 36.27 **ATOM** 1636 CB VAL 371 67.885 24.097 21.046 1.00 36.15 **ATOM** 1637 CG1 VAL 371 66.600 24.487 21.758 1.00 32.69 **ATOM** 1638 CG2 VAL 371 67.612 23.892 19.567 1.00 33.75 **ATOM** 1639 C VAL 371 69.196 25.423 22.745 1.00 41.55 VAL **ATOM** 1640 O 371 68.638 26.367 23.316 1.00 40.82 **ATOM** 1641 N THR 372 70.018 24.581 23.378 1.00 40.42 **ATOM** 1642 CA THR 372 70.300 24.733 24.804 1.00 41.69 **ATOM** 1643 CB THR 372 71.037 23.499 25.397 1.00 42.36 372 **ATOM** 1644 OG1 THR 72.125 23.133 24.548 1.00 53.57 **ATOM** 1645 CG2 THR 372 70.090 22.313 25.523 1.00 43.54 **ATOM** 1646 C THR 372 71.090 26.021 25.048 1.00 38.75 **ATOM** 1647 O THR 372 70.858 26.714 26.042 1.00 37.51 **ATOM** 1648 N **ASP** 373 71.987 26.360 24.122 1.00 36.73 **ATOM** 1649 CA ASP 373 72.768 27.594 24.223 1.00 30.96

ATOM 1650 CB ASP 373 73.741 27.732 23.047 1.00 31.26 ATOM 1651 CG ASP 373 74.865 26.707 23.085 1.00 35.85 **ATOM** 1652 OD1 ASP 373 75.523 26.508 22.042 1.00 36.73 **ATOM** 1653 OD2 ASP 373 75.102 26.103 24.153 1.00 39.92 1654 C **ATOM ASP** 373 71.797 28.769 24.230 1.00 31.30 **ATOM** 1655 O- ASP 373 71.926 29.689 25.039 1.00 35.37 1656 N **ATOM** LEU 374 70.804 28.711 23.348 1.00 27.72 ATOM 1657 CA LEU 374 69.783 29.751 23.257 1.00 28.18 **ATOM** 1658 CB LEU 374 68.881 29.521 22.042 1.00 28.41 **ATOM** 1659 CG LEU 374 69.391 30.055 20.703 1.00 29.87 **ATOM** 1660 CD1 LEU 374 68.533 29.520 19.563 1.00 25.44 **ATOM** 1661 CD2 LEU 374 69.385 31.581 20.728 1.00 23.74 ATOM 1662 C LEU 374 68.946 29.786 24.527 1.00 28.61 **ATOM** 1663 O LEU 374 68.516 30.859 24.968 1.00 29.51 375 **ATOM** 1664 N ARG 68.690 28.615 25.105 1.00 32.32 **ATOM** 1665 CA ARG 375 67.925 28.532 26.345 1.00 33.19 ATOM 1666 CB ARG 375 67.758 27.074 26.776 1.00 41.70 **ATOM** 1667 CG ARG 375 66.360 26.524 26.609 1.00 51.03 **ATOM** 1668 CD ARG 375 65.979 26.416 25.153 1.00 60.16 1669 NE ARG ATOM 375 64.648 25.840 24.987 1.00 74.28 1670 CZ ARG **ATOM** 375 64.324 24.587 25.296 1.00 79.34 **ATOM** 1671 NH1 ARG 375 65.233 23.756 25.796 1.00 80.84 **ATOM** 1672 NH2 ARG 375 63.084 24.157 25.092 1.00 77.44 **ATOM** 1673 C ARG 375 68.692 29.296 27.423 1.00 32.02 **ATOM** 1674 O **ARG** 375 68.132 30.150 28.108 1.00 30.42 ATOM 1675 N **MET** 376 69.993 29.020 27.521 1.00 32.30 1676 CA MET **ATOM** 376 70.860 29.668 28.499 1.00 36.82 1677 CB MET **ATOM** 376 72.278 29.097 28.433 1.00 45.36 **ATOM** 1678 CG MET 376 72.375 27.645 28.866 1.00 66.71 ATOM 1679 SD MET 376 74.078 27.057 28.966 1.00 89.64 ATOM 1680 CE MET 376 74.256 26.229 27.400 1.00 85.51 **ATOM** 1681 C **MET** 376 70.880 31.182 28.310 1.00 37.49 376 **ATOM** 1682 O **MET** 70.780 31.928 29.281 1.00 39.99 **ATOM** 1683 N ILE 377 71.008 31.630 27.060 1.00 33.14 ATOM 1684 CA ILE 377 71.009 33.057 26.740 1.00 25.98 **ATOM** 1685 CB ILE 377 71.181 33.291 25.211 1.00 22.79 1686 CG2 ILE 377 ATOM 70.838 34.727 24.834 1.00 25.29 **ATOM** 1687 CG1 ILE 377 72.606 32.947 24.785 1.00 21.42 ATOM 1688 CD1 ILE 377 72.816 32.971 23.282 1.00 19.37 **ATOM** 1689 C ILE 377 69.690 33.664 27.228 1.00 27.11 **ATOM** 1690 O ILE 377 69.676 34.727 27.856 1.00 28.09 **ATOM** 1691 N GLY 378 68.584 32.969 26.975 1.00 29.34 1692 CA GLY **ATOM** 378 67.292 33.457 27.418 1.00 30.41 **ATOM** 1693 C GLY 378 67.233 33.532 28.934 1.00 36.85 66.672 34.481 29.489 1.00 36.44 1694 O **GLY** 378 **ATOM ATOM** 1695 N ALA 379 67.837 32.547 29.603 1.00 37.98 67.869 32.483 31.066 1.00 36.44 ATOM 1696 CA ALA 379

ATOM 1697 CB ALA 68.415 31.133 31.528 1.00 35.63 379 **ATOM** 1698 C ALA 379 68.712 33.613 31.642 1.00 34.14 **ATOM** 1699 O ALA 379 68.259 34.343 32.523 1.00 35.15 **ATOM** 1700 N CYA 69.941 33.747 31.144 1.00 36.66 380 **ATOM** 1701 CA CYA 380 70.860 34.795 31.587 1.00 37.27 **ATOM** 1702 CB CYA 72.172 34.728 30.810 1.00 36.85 380 **ATOM** 1703 SG CYA 380 73.201 33.338 31.250 1.00 52.80 **ATOM** 1704 AS CYA 380 74.942 33.593 29.823 1.00 65.79 **ATOM** 1705 C CYA 380 70.230 36.165 31.398 1.00 38.70 **ATOM** 1706 O CYA 70.337 37.033 32.270 1.00 45.73 380 **ATOM** 1707 N HIS 381 69.555 36.354 30.265 1.00 37.32 **ATOM** 1708 CA HIS 381 68.906 37.623 29.994 1.00 32.11 **ATOM** 1709 CB HIS 381 68.377 37.687 28.565 1.00 25.76 **ATOM** 1710 CG HIS 381 67.596 38.932 28.285 1.00 20.30 **ATOM** 1711 CD2 HIS 381 67.998 40.200 28.044 1.00 16.31 **ATOM** 1712 ND1 HIS 381 66.218 38.971 28.336 1.00 22.06 **ATOM** 1713 CE1 HIS 65.807 40.210 28.146 1.00 21.20 381 **ATOM** 1714 NE2 HIS 381 66.869 40.976 27.968 1.00 22.58 **ATOM** 1715 C HIS 381 67.773 37.893 30.980 1.00 32.68 **ATOM** 1716 O HIS 381 67.602 39.024 31.431 1.00 33.38 **ATOM** 1717 N ALA 382 66.982 36.873 31.296 1.00 31.27 ATOM 1718 CA ALA 382 - 65.884 37.045 32.243 1.00 29.39 ATOM 1719 CB ALA 382 65.121 35.742 32.409 1.00 25.18 **ATOM** 1720 C ALA 382 66.420 37.531 33.596 1.00 34.32 **ATOM** 1721 O ALA 382 65.902 38.501 34.160 1.00 37.79 **ATOM** 1722 N SER 383 67.483 36.893 34.085 1.00 36.88 **ATOM** 1723 CA SER 383 68.100 37.268 35.361 1.00 39.74 **ATOM** 1724 CB SER 383 69.233 36.297 35.719 1.00 42.58 **ATOM** 1725 OG SER 383 68.734 35.010 36.049 1.00 61.85 ATOM 1726 C SER 383 68.638 38.697 35.311 1.00 36.49 **ATOM** 1727 O **SER** 383 68.443 39.480 36.243 1.00 43.81 69.305 39.036 34.213 1.00 33.66 **ATOM** 1728 N ARG 384 **ATOM** 1729 CA ARG 384 69.866 40.367 34.043 1.00 35.39 1730 CB ARG **ATOM** 384 70.800 40.404 32.835 1.00 29.29 **ATOM** 1731 CG ARG 384 71.590 41.679 32.731 1.00 29.20 **ATOM** 1732 CD ARG 384 72.881 41.435 31.995 1.00 37.73 ATOM 1733 NE ARG 384 73.657 42.663 31.850 1.00 48.97 **ATOM** 1734 CZ ARG 384 74.346 43.245 32.826 1.00 45.41 **ATOM** 1735 NH1 ARG 384 74.371 42.715 34.038 1.00 44.51 1736 NH2 ARG 384 **ATOM** 75.008 44.368 32.584 1.00 41.43 **ATOM** 1737 C ARG 384 68.777 41.431 33.916 1.00 39.45 **ATOM** 1738 O **ARG** 384 68.913 42.537 34.444 1.00 44.47 1739 N PHE 385 **ATOM** 67.673 41.077 33.270 1.00 36.42 1740 CA PHE 385 ATOM 66.568 42.007 33.099 1.00 34.68 **ATOM** 1741 CB PHE 385 65.444 41.393 32.262 1.00 30.21 1742 CG PHE **ATOM** 385 64.263 42.304 32.081 1.00 29.48 **ATOM** 1743 CD1 PHE 385 64.289 43.313 31.127 1.00 29.70

ATOM	1744 CD2 PHE 385	63.130 42.161 32.873 1.00 28.04
ATOM	1745 CE1 PHE 385	63.203 44.169 30.966 1.00 33,50
ATOM	1746 CE2 PHE 385	62.040 43.012 32.718 1.00 31.35
ATOM		62.077 44.017 31.763 1.00 32.08
ATOM	1748 C PHE 385	66.040 42.412 34.468 1.00 35.76
ATOM	1749 O- PHE 385	65.761 43.590 34.693 1.00 40.58
ATOM	1750 N LEU 386	65.906 41.441 35.373 1.00 37.55
ATOM	1751 CA LEU 386	65.429 41.706 36.735 1.00 41.01
ATOM	1751 CR LEU 386	65.394 40.413 37.563 1.00 42.30
ATOM	1752 CB LEU 386	64.240 39.434 37.317 1.00 43.34
ATOM	1754 CD1 LEU 386	64.559 38.066 37.912 1.00 43.50
ATOM	1755 CD2 LEU 386	62.946 39.992 37.899 1.00 44.01
ATOM	1755 CD2 EEU 386	66.342 42.735 37.405 1.00 40.08
ATOM	1757 O LEU 386	
ATOM		67.643 42.613 37.153 1.00 34.86
ATOM		68.631 43.537 37.700 1.00 39.09
ATOM	1760 CB HIS 387	70.046 43.034 37.421 1.00 39.99
ATOM	1761 CG HIS 387	70.402 41.791 38.172 1.00 56.37
ATOM	1762 CD2 HIS 387	71.384 40.881 37.974 1.00 60.11
ATOM	1763 ND1 HIS 387	69.711 41.370 39.290 1.00 60.40
ATOM	1764 CE1 HIS 387	70.252 40.255 39.746 1.00 61.89
ATOM	1765 NE2 HIS 387	71.269 39.937 38.966 1.00 63.96
ATOM	1766 C HIS 387	68.446 44.928 37.101 1.00 41.00
ATOM	1767 O HIS 387	68.492 45.927 37.817 1.00 46.99
ATOM	1768 N MET 388	68.213 44.982 35.792 1.00 39.15
ATOM	1769 CA MET 388	
ATOM	1770 CB MET 388	67.676 45.992 33.612 1.00 35.12
ATOM	1771 CG MET 388	68.810 45.442 32.753 1.00 37.24
ATOM	1772 SD MET 388	68.259 45.150 31.051 1.00 41.75
ATOM	1773 CE MET 388	69.274 43.748 30.573 1.00 35.23
ATOM	1774 C MET 388	66.880 47.048 35.733 1.00 36.52
ATOM	1775 O MET 388	66.994 48.265 35.888 1.00 43.39
ATOM		65.792 46.371 36.103 1.00 38.05
ATOM	1777 CA LYS 389	64.637 47.025 36.729 1.00 42.88
ATOM	1778 CB LYS 389	63.481 46.035 36.866 1.00 47.83
ATOM	1779 CG LYS 389	62.835 45.627 35.560 1.00 52.36
ATOM	1780 CD LYS 389	62.040 44.340 35.731 1.00 61.84
ATOM	1781 CE LYS 389	60.978 44.451 36.814 1.00 69.04
ATOM	1782 NZ LYS 389	60.254 43.162 36.987 1.00 70.00
ATOM	1783 C LYS 389	64.983 47.587 38.107 1.00 43.99
ATOM	1784 O LYS 389	64.455 48.621 38.525 1.00 44.22
ATOM	1785 N VAL 390	65.851 46.878 38.816 1.00 45.50
ATOM	1786 CA VAL 390	66.290 47.286 40.142 1.00 47.76
ATOM	1787 CB VAL 390	67.152 46.186 40.804 1.00 46.30
ATOM	1788 CG1 VAL 390	67.796 46.706 42.079 1.00 49.20
ATOM	1789 CG2 VAL 390	66.305 44.962 41.097 1.00 42.69
ATOM	1790 C VAL 390	67.109 48.571 40.070 1.00 47.25
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ATOM 1791 O VAL 390 66.811 49.540 40.760 1.00 48.67 **ATOM** 1792 N **GLU** 391 68.115 48.580 39.199 1.00 44.11 **ATOM** 1793 CA GLU 391 69.009 49.721 39.047 1.00 45.79 **ATOM** 1794 CB GLU 391 70.266 49.311 38.273 1.00 45.78 **ATOM** 1795 CG GLU 391 70.998 48.091 38.830 1.00 57.29 **ATOM** 1796 CD GLU 391 71.479 48.268 40.261 1.00 61.20 **ATOM** 1797 OE1 GLU 391 71.845 49.400 40.646 1.00 57.29 **ATOM** 1798 OE2 GLU 391 71.496 47.263 41.001 1.00 63.69 **ATOM** 1799 C GLU 391 68.410 50.959 38.391 1.00 49.16 **ATOM** 1800 O GLU 391 68.463 52.055 38.956 1.00 58.82 **ATOM** 1801 N CYA 392 67.802 50.782 37.224 1.00 49.75 1802 CA CYA ATOM 392 67.255 51.908 36.475 1.00 45.56 1803 CB CYA 392 ATOM 67.667 51.768 35.016 1.00 44.82 **ATOM** 1804 SG CYA 392 69.443 51.771 34.913 1.00 50.78 **ATOM** 1805 AS CYA 392 69.929 50.778 33.022 1.00 53.29 **ATOM** 1806 C CYA 392 65.771 52.200 36.601 1.00 44.35 **ATOM** 1807 O CYA 392 64.988 51.324 36.962 1.00 44.10 **ATOM** 1808 N PRO 393 65.378 53.469 36.365 1.00 45.52 **ATOM** 1809 CD PRO 393 66.275 54.603 36.075 1.00 37.38 **ATOM** 1810 CA PRO 393 63.982 53.916 36.444 1.00 45.41 **ATOM** 1811 CB PRO 393 64.105 55.438 36.376 1.00 43.33 **ATOM** 1812 CG PRO 393 65.329 55.644 35.542 1.00 39.89 ATOM 1813 C PRO 393 63.108 53.376 35.318 1.00 44.89 393 **ATOM** 1814 O PRO 63.556 53.239 34.175 1.00 45.60 **ATOM** 1815 N THR 394 61.843 53.135 35.647 1.00 47.52 **ATOM** 1816 CA THR 394 60.853 52.603 34.713 1.00 53.06 **ATOM** 1817 CB THR 394 59.459 52.583 35.371 1.00 61.06 **ATOM** 1818 OG1 THR 394 59.609 52.470 36.794 1.00 72.44 **ATOM** 1819 CG2 THR 394 58.640 51.401 34.860 1.00 61.05 **ATOM** 1820 C THR 394 60.767 53.373 33.392 1.00 49.98 1821 O THR 394 **ATOM** 60.507 52.786 32.339 1.00 51.06 **GLU** 395 **ATOM** 1822 N 61.024 54.676 33.452 1.00 48.55 1823 CA GLU **395**. **ATOM** 60.970 55.548 32.282 1.00 44.21 1824 CB GLU **ATOM** 395 61.258 56.987 32.697 1.00 41.66 **ATOM** 1825 C GLU 395 61.899 55.134 31.134 1.00 43.46 1826 O GLU 395 ATOM 61.684 55.527 29.988 1.00 44.17 1827 N LEU 396 **ATOM** 62.934 54.359 31.449 1.00 41.05 1828 CA LEU 396 **ATOM** 63.898 53.899 30.448 1.00 39.55 1829 CB LEU 396 65.270 53.708 31.106 1.00 35.03 **ATOM ATOM** 1830 CG LEU 396 66.296 54.834 30.945 1.00 40.06 1831 CD1 LEU 396 65.638 56.200 31.055 1.00 39.06 **ATOM** 1832 CD2 LEU 396 67.398 54.669 31.978 1.00 32.78 **ATOM ATOM** 1833 C LEU 396 63.468 52.602 29.757 1.00 38.50 1834 O LEU **ATOM** 396 64.106 52.150 28.804 1.00 34.72 **ATOM** 1835 N PHE 397 62.364 52.028 30.225 1.00 38.76 **ATOM** 1836 CA PHE 397 61.860 50.774 29.683 1.00 36.57 **ATOM** 1837 CB PHE 397 61.610 49.775 30.819 1.00 33.96

ATOM 1838 CG PHE 397 62.842 49.421 31.607 1.00 36.95 **ATOM** 1839 CD1 PHE 397 63.331 50.280 32.587 1.00 34.61 **ATOM** 1840 CD2 PHE 397 63.523 48.234 31.362 1.00 37.14 **ATOM** 1841 CE1 PHE 397 64.481 49.964 33.310 1.00 31.57 **ATOM** 1842 CE2 PHE 397 64.675 47.908 32.082 1.00 37.85 **ATOM** 1843 CZ PHE 397 65.153 48.776 33.056 1.00 33.08 **ATOM** 1844 C PHE 397 60.584 50.921 28.858 1.00 35.65 **ATOM** 1845 O PHE 397 59.519 51.249 29.399 1.00 35.75 **ATOM** 1846 N PRO 398 60.672 50.685 27.536 1.00 35.78 **ATOM** 1847 CD PRO 398 61.891 50.367 26.767 1.00 32.81 **ATOM** 1848 CA PRO 398 59.503 50.786 26.658 1.00 33.94 ATOM 1849 CB PRO 398 60.041 50.297 25.315 1.00 33.91 **ATOM** 1850 CG PRO 398 61.488 50.707 25.356 1.00 33.09 **ATOM** 1851 C PRO 398 58.434 49.840 27.210 1.00 34.98 **ATOM** 1852 O PRO 398 58.753 48.729 27.654 1.00 35.76 **ATOM** 1853 N PRO 399 57.163 50.267 27.219 1.00 37.67 1854 CD PRO **ATOM** 399 56.661 51.578 26.776 1.00 38.02 **ATOM** 1855 CA PRO 399 56.070 49.433 27.733 1.00 36.86 **ATOM** 1856 CB PRO 399 54.803 50.183 27.291 1.00 34.14 **ATOM** 1857 CG PRO 399 55.282 51.240 26.310 1.00 37.00 ATOM 1858 C **PRO** 399 56.085 47.970 27.273 1.00 37.06 **ATOM** 1859 O **PRO** 399 55.967 47.063 28.099 1.00 37.07 56.299 47.738 25.980 1.00 35.13 **ATOM** 1860 N LEU 400 1861 CA LEU **ATOM** 400 56.327 46.374 25.445 1.00 35.86 1862 CB LEU 56.314 46.385 23.914 1.00 31.49 **ATOM** 400 **ATOM** 1863 CG LEU 400 56.181 45.017 23.227 1.00 30.73 **ATOM** 1864 CD1 LEU 400 54.901 44.330 23.674 1.00 21.35 **ATOM** 1865 CD2 LEU 400 56.197 45.183 21.720 1.00 25.42 **ATOM** 1866 C LEU 400 57.542 45.597 25.958 1.00 36.51 **ATOM** 1867 O LEU 400 57.458 44.392 26.219 1.00 37.47 1868 N PHE **ATOM** 401 58.671 46.290 26.095 1.00 32.26 **ATOM** 1869 CA PHE 401 59.899 45.682 26.596 1.00 35.15 **ATOM** 1870 CB PHE 401 61.014 46.739 26.648 1.00 35.99 **ATOM** 1871 CG PHE 401 62.346 46.213 27.117 1.00 39.41 **ATOM** 1872 CD1 PHE 401 62.845 45.003 26.639 1.00 35.94 **ATOM** 1873 CD2 PHE 401 63.119 46.944 28.019 1.00 40.55 **ATOM** 1874 CE1 PHE 401 64.088 44.531 27.055 1.00 30.16 401 **ATOM** 1875 CE2 PHE 64.367 46.478 28.439 1.00 35.53 1876 CZ PHE **ATOM** 401 64.849 45.271 27.952 1.00 36.39 **ATOM** 1877 C PHE 401 59.607 45.129 27.996 1.00 36.42 **ATOM** 1878 O PHE 401 59.957 43.995 28.317 1.00 36.71 1879 N LEU **ATOM** 402 58.920 45.925 28.805 1.00 36.59 **ATOM** 1880 CA LEU 402 58.561 45.528 30.158 1.00 37.68 **ATOM** 1881 CB LEU 402 57.986 46.720 30.917 1.00 40.71 **ATOM** 1882 CG LEU 402 58.963 47.751 31.463 1.00 43.13 **ATOM** 1883 CD1 LEU 402 58.180 48.926 32.031 1.00 39.88 **ATOM** 1884 CD2 LEU 402 59.847 47.103 32.527 1.00 38.39

ATOM 1885 C LEU 402 57.521 44.420 30.164 1.00 38.02 **ATOM** 1886 O LEU 402 57.582 43.507 30.984 1.00 37.39 **ATOM** 1887 N GLU 403 56.558 44.522 29.251 1.00 39.74 1888 CA GLU **ATOM** 403 55.469 43.559 29.166 1.00 42.79 **ATOM** 1889 CB GLU 403 54.445 44.022 28.129 1.00 46.21 **ATOM** 1890 CG GLU 403 53.092 43.330 28.232 1.00 56.88 **ATOM** 1891 CD GLU 403 52.090 43.833 27.202 1.00 65.21 **ATOM** 1892 OE1 GLU 403 52.230 44.983 26.728 1.00 70.60 **ATOM** 1893 OE2 GLU 403 51.154 43.073 26.870 1.00 70.53 **ATOM** 1894 C GLU 403 55.890 42.121 28.886 1.00 40.14 ATOM 1895 O GLU 403 55.368 41.200 29.506 1.00 40.57 1896 N VAL **ATOM** 404 56.835 41.932 27.966 1.00 39.43 1897 CA VAL 404 **ATOM** 57.292 40.586 27.610 1.00 40.96 **ATOM** 1898 CB VAL 404 57.851 40.516 26.159 1.00 35.50 **ATOM** 1899 CG1 VAL 404 56.807 40.995 25.177 1.00 43.46 **ATOM** 1900 CG2 VAL 404 59.132 41.321 26.030 1.00 25.74 ATOM 1901 C VAL 404 58.317 39.946 28.536 1.00 41.94 **ATOM** 1902 O VAL 404 58.468 38.722 28.533 1.00 43.82 **ATOM** 1903 N PHE 405 59.026 40.759 29.310 1.00 39.84 **ATOM** 1904 CA PHE 405 60.051 40.223 30.189 1.00 42.73 **ATOM** 1905 CB PHE 405 61.401 40.897 29.913 1.00 36.85 **ATOM** 405 1906 CG PHE 61.963 40.596 28.551 1.00 33.23 **ATOM** 1907 CD1 PHE 405 62.283 41.625 27.672 1.00 33.90 1908 CD2 PHE 405 ATOM 62.157 39.281 28.138 1.00 31.62 **ATOM** 1909 CE1 PHE 405 62.786 41.351 26.399 1.00 39.16 **ATOM** 1910 CE2 PHE 405 62.657 38.997 26.872 1.00 33.33 1911 CZ PHE 405 62.972 40.033 25.999 1.00 31.99 **ATOM** 1912 C PHE ATOM 405 59.723 40.273 31.676 1.00 43.97 **ATOM** 1913 O PHE 405 60.636 39.943 32.460 1.00 46.56 **ATOM** 1 01 HOH 501 67.928 36.755 11.188 1.00 33.04 **ATOM** 2 O1 HOH 502 69.618 40.719 13.009 1.00 23.00 ATOM 3 O1 HOH 503 64.885 40.168 12.340 1.00 23.00 **ATOM** 4 O1 HOH 504 63.079 40.108 15.841 1.00 23.00 63.404 46.536 15.354 1.00 36.41 **ATOM** 5 O1 HOH 505 506 **ATOM** 6 O1 HOH 61.299 15.617 -0.595 1.00 23.00 **ATOM** 7 O1 HOH 507 67.359 15.375 0.551 1.00 23.00 **ATOM** 8 O1 HOH 508 67.230 12.002 -0.634 1.00 23.00 **ATOM** 9 O1 HOH 509 66.906 12.467 3.855 1.00 23.00 **ATOM** 10 O1 HOH 510 61.785 9.946 3.983 1.00 23.00 **ATOM** 11 O1 HOH 511 57.670 11.385 9.909 1.00 23.00 **ATOM** O1 HOH 512 55.791 11.570 10.291 1.00 23.00 **ATOM** O1 HOH 513 13 54.637 14.058 9.201 1.00 23.00 **ATOM** 14 O1 HOH 514 55.882 16.054 12.204 1.00 26.53 **ATOM** 515 15 O1 HOH 53.685 15.842 18.209 1.00 23.00 **ATOM** 16 O1 HOH 516 49.559 24.773 19.020 1.00 23.00 **ATOM** 17 O1 HOH 517 51.258 25.512 13.384 1.00 37.74 **ATOM** 18 O1 HOH 518 53.551 25.749 10.593 1.00 42.31

	ATOM	· 19 C	о нон	519	50.338 23	3.299 7.662	2 1.00 41.19
	ATOM	20 C	1 HOH	520		0.272 8.323	
	ATOM	21 C	1 HOH	521	48.630 20	0.291 6.429	
	ATOM	22 C	1 HOH	522	49.233 17	7.389 2.867	
	ATOM	23 C	1 HOH	523		2.770 1.260	
	ATOM	24 C	нон 1	524		3.621 -1.020	
	ATOM	25 O	1 HOH	525		.509 2.147	
	ATOM	26 O	1 HOH	526		5.071 2.268	
	ATOM	27 O	1 HOH	527		6.025 6.809	
	ATOM	28 O	1 HOH	528		.399 6.419	
	ATOM	29 O	1 HOH	529		.811 9.409	
	ATOM	30 O	1 HOH			.056 13.590	
	ATOM	31 O	1 HOH	531		.824 10.638	
	ATOM	32 O	1 HOH	532		.867 13.186	· · ·
	ATOM	33 O	1 HOH	533		.774 10.959	
	ATOM	34 O	1 HOH	534		.032 19.560	
	ATOM	35 O	1 HOH	535		.757 24.168	
	ATOM	36 O	1 HOH	536		.330 31.881	
	ATOM	37 O	1 HOH	537	62.563 49.	.327 37.804	· -
	ATOM	38 O	1 HOH	538	61.736 40.	.280 35.059	
	ATOM	39 O	1 HOH	539		.155 34.156	
	ATOM	40 O	HOH 1	540	61.872 35.	.187 29.990	
	ATOM	41 O	HOH	541	63.701 36.	808 28.720	
	ATOM	42 O	HOH I	542	62.255 35.	864 26.425	1.00 26.69
	ATOM	43 O	HOH	543	63.567 33.	453 25.308	
	ATOM	44 O1	HOH	544	65.456 30.	135 27.713	1.00 23.00
	ATOM	45 O1		545	61.997 26.	566 24.157	1.00 23.00
	ATOM	46 O1	HOH	546	61.422 22.	231 24.358	1.00 23.00
	ATOM	47 O1		547	59.636 21.	462 25.378	1.00 23.00
	ATOM	48 O1		548	64.860 21.	210 22.578	1.00 23.00
	ATOM	49 O1		549	63.316 14.9	964 15.508	1.00 52.55
	ATOM	50 O1		550		707 15.710	1.00 48.78
	ATOM	51 01		551		565 12.081	1.00 23.00
	ATOM	52 O1		552			1.00 23.00
	ATOM	53 O1		553	68.086 12.8		1.00 23.00
	ATOM	54 01		554	69.504 11.9		1.00 23.00
	ATOM	55 O1		555	72.311 15.1		1.00 23.00
	ATOM	56 O1		556	74.716 15.1		1.00 23.00
	ATOM	57 O1		557	73.109 17.9		1.00 23.00
	ATOM	58 O1		558	71.316 15.4		1.00 23.00
	ATOM	59 01	НОН	559	74.717 14.5		1.00 23.00
	ATOM	60 O1	НОН	560	73.523 22.3		1.00 23.00
	ATOM	61 01	НОН	561	76.491 23.0		1.00 51.34
	ATOM	62 01	НОН	562	73.961 29.8		1.00 33.87
	ATOM	63 01		563	76.164 33.0		1.00 23.00
	ATOM	64 01		564	77.193 34.0		1.00 37.14
1	ATOM	65 O1	HOH	565	76.525 41.3	395 10.460	1.00 23.00

ATOM	66	01	НОН	566	79.358 49.535 15.048 1.00 53.78
ATOM	67	O1		567	78.046 53.530 9.188 1.00 23.00
ATOM	68	01	НОН	568	68.058 52.158 15.548 1.00 23.00
ATOM	69	01	НОН	569	68.598 53.164 18.083 1.00 45.72
ATOM	70	01	HOH	570	73.482 58.914 21.552 1.00 58.99
ATOM	71	01	HOH	571	65.648 53.551 26.240 1.00 23.00
ATOM	72	01	HOH	572	75.776 46.207 30.367 1.00 33.32
ATOM	73	01	HOH	573	78.686 46.470 31.087 1.00 23.00
ATOM	74	01	HOH	574	77.580 41.209 31.884 1.00 23.00
ATOM	75		HOH	575	76.879 31.531 24.067 1.00 23.00
ATOM	76			576	77.927 29.163 20.647 1.00 23.00
ATOM	77	01	HOH	577	80.180 24.963 17.233 1.00 53.36
ATOM	78		HOH	578	80.631 25.802 15.508 1.00 23.00
ATOM	79	01	HOH	579	82.104 22.566 14.156 1.00 23.00
ATOM	80	01	HOH	580	76.954 22.077 18.425 1.00 46.50
ATOM	81	01	HOH	581	86.619 37.903 16.945 1.00 47.66
ATOM	82	01	HOH	582	83.586 42.305 18.576 1.00 23.00
ATOM	83	01	HOH	583	83.481 45.262 19.526 1.00 23.00
ATOM	84	01	НОН	584	66.787 32.864 33.796 1.00 23.00
ATOM	85	01	HOH	585	59.447 33.572 30.734 1.00 23.00
ATOM	86	01	HOH	586	57.013 32.278 31.125 1.00 23.00
ATOM	87	01	нон	587	58.084 29.428 24.648 1.00 24.06
ATOM	88	01	НОН	588	52.774 25.054 32.650 1.00 57.81
ATOM	89	01	НОН	589	53.800 24.465 34.834 1.00 23.00
ATOM	90	01	НОН	590	47.195 30.205 30.414 1.00 23.00
ATOM	91	01	НОН	591	48.978 35.051 30.228 1.00 23.00
ATOM	92	01	НОН	592	49.280 39.962 31.041 1.00 23.00
ATOM	93	01	НОН	593	42.329 32.230 20.993 1.00 23.00
ATOM	94	01	НОН	594	44.199 32.910 19.088 1.00 23.00
ATOM	95	01	НОН	595	41.542 27.336 19.178 1.00 23.00
ATOM	96	01	HOH	596	48.971 31.296 14.022 1.00 23.00
ATOM	97	01	HOH	597	50.180 31.092 7.307 1.00 23.00
ATOM			HOH		64.465 28.209 3.208 1.00 45.35
ATOM			HOH	599	67.740 26.910 1.986 1.00 23.00
ATOM	100	01	HOH	600	67.958 31.203 3.532 1.00 23.00
ATOM ATOM	101	01	HOH	601	68.885 22.721 0.234 1.00 39.53
ATOM	102 103		HOH	602	46.735 20.335 25.877 1.00 44.92
ATOM			HOH		47.359 19.644 28.494 1.00 41.57 52.555 20.000 24.632 1.00 48.75
		C	ACY		52.555 39.909 24.622 1.00 48.75
ATOM ATOM	2301	0 0	ACY	701	52.351 40.361 25.771 1.00 48.92
	2302		T ACY		53.503 39.156 24.279 1.00 50.69
ATOM			3 ACY		51.543 40.314 23.527 1.00 41.32
ATOM ATOM	2304 2305		IBR	1	67.309 42.207 18.510 1.00 32.20 68.705 43.104 23.237 1.00 20.50
ATOM			IBR	1	68.795 43.194 23.237 1.00 29.59
ATOM	2306	C4			67.192 43.467 19.068 1.00 25.49
ATOM	2307 2308		IBR	1	69.096 44.270 24.011 1.00 25.67
VI O'M	2300	CJ	TDK.	1	67.884 43.772 20.218 1.00 35.08

				4.1				
ATOM	2309	C6	IBR	1	68.489	44.345	25.356	1.00 30.87
ATOM	2310	· C7	IBR	• 1	68.673	42.828	20.790	1.00 30.76
ATOM	2311	C8	IBR	1	67.681	43.327	25.704	1.00 29.18
ATOM	2312	C9	IBR	1	68.811	41.580	20.269	1.00 32.19
ATOM	2313	C10	IBR	1	67.383	42.244	24.921	1.00 26.78
ATOM	2314	C11	IBR	1	68.122	41.241	19.099	
ATOM	2315	C12	IBR	1	67.979	42.171	23.609	1.00 24.47
ATOM	2316	C13	IBR	1	66.529	41.932	17.285	1.00 17.69
ATOM	2317	C14	IBR	- 1	68.730	45.450	26.287	1.00 30.43
ATOM	2318	C15	IBR	1	67.011	40.785	16.271	1.00 21.37
ATOM	2319	C16	IBR	1	67.939	46.867	25.912	1.00 23.75
ATOM	2320	C17	IBR	1	65.946	40.598	15.151	1.00 23.91
ATOM	2321	C18	IBR	1	70.126	46.087	26.069	1.00 26.02
ATOM	2322	BR1	IBR	1	67.708	45.504	20.878	1.00 34.64
ATOM	2323	BR2	IBR	1	69.927	40.301	21.039	1.00 32.01
ATOM	2324	N1	IBR	1	68.284	40.938	15.821	1.00 18.75
ATOM	2325	O 1	IBR	1	67.068	43.397	26.981	1.00 26.31
ATOM	2326	O2	IBR ·	1	69.393	43.153	21.933	1.00 30.15
ATOM	2327	O3	IBR	1	66.368	40.592	14.004	1.00 23.29
ATOM	2328	O4	IBR	1	64.786	40.511	15.515	1.00 23.47
END				•				
END				•				

APPENDIX 6

TR_T3.PDB

REMARK rTR t3 full length numbering **REMARK** REMARK Rfactor 0.221 Rfree 0.240 REMARK Resolution 5. 2.0 all reflections REMARK conformation of MET 388 confirmed by SA omit map REMARK REMARK Three cacodylate-modified cysteines (CYA) REMARK Cya334, Cya380, Cya392 REMARK cacodylate modeled as single arsenic atom REMARK REMARK side chain of certain residues modeled as ALA due to poor density; REMARK however, residue name reflects true residue for clarity **REMARK** REMARK clone obtained from Murray et. al. REMARK deposited sequence confirmed, REMARK differing from that reported by Thompson et. al. REMARK in the following codons: REMARK 281 Thr - Ala REMARK 285 Lys - Glu REMARK identical to that reported by Mitsuhashi et. al. REMARK gb:RNTRAVI X07409 JRNL AUTH M.B. MURRAY, N.D.ZILZ, N.L.MCCREARY, M.J.MACDONALD JRNL **AUTH 2 H.C.TOWLE** JRNL TITL ISOLATION AND CHARACTERIZATION OF RAT CDNA CLONES FOR TWO JRNL TITL 2 DISTINCT THYROID HORMONE RECPTORS JRNL REF **JBC** V. 263 25 1988 JRNL AUTH C.C.THOMPSON, C.WEINBERGER, R.LEBO, R.M.EVANS TITL IDENTIFICATION OF A NOVEL THYROID HORMONE RECEPTOR JRNL **EXPRESSED** JRNL TITL 2 IN THE MAMMALIAN CENTRAL NERVOUS SYSTEM JRNL REF SCIENCE V. 237 1987 AUTH T.MITSUHASHI, G. TENNYSON, V. NIKODEM JRNL JRNL NUCLEOTIDE SEQUENCE OF NOVEL CDNAS GENERATED BY **ALTERNATIVE** TITL 2 SPLICING OF A RAT THYROID HORMONE RECEPTOR GENE JRNL TRANSCRIPT JRNL REF NUC. ACIDS. RES. V. 16 12 1988 REMARK ATOM 1 CB ARG 157 68.406 10.620 7.027 1.00 41.66 ATOM 2 CG ARG 157 69.926 10.540 6.997 1.00 44.48 ATOM 3 CD ARG 157 70.552 11.261 8.173 1.00 47.02

70.112 10.680 9.435 1.00 49.73

21388546 277

4 NE ARG 157

ATOM

ATOM	·· 5 CZ ARG 157	70.917 10.392 10.450 1.00 51.21
ATOM	6 NH1 ARG 157	72.223 10.629 10.361 1.00 51.79
ATOM	7 NH2 ARG 157	70.405 9.871 11.556 1.00 51.92
ATOM	8 C ARG 157	66.308 9.993 5.774 1.00 36.48
ATOM	9 O ARG 157	66.047 10.318 4.622 1.00 38.84
ATOM	10 N ARG 157	68.479 9.473 4.839 1.00 41.22
ATOM	11 CA ARG 157	67.734 9.580 6.135 1.00 39.98
ATOM	12 N PRO 158	65.366 9.953 6.728 1.00 33.85
ATOM	13 CD PRO 158	65.494 9.553 8.139 1.00 34.72
ATOM	14 CA PRO 158	63.981 10.336 6.407 1.00 31.89
ATOM	15 CB PRO 158	63.219 10.015 7.694 1.00 31.87
ATOM	16 CG PRO 158	64.260 10.158 8.759 1.00 33.55
ATOM	17 C PRO 158	63.758 11.783 5.947 1.00 29.77
ATOM	18 O PRO 158	64.221 12.739 6.575 1.00 27.93
ATOM	19 N GLU 159	63.071 11.918 4.819 1.00 26.20
ATOM	20 CA GLU 159	62.759 13.217 4.239 1.00 24.07
ATOM	21 CB GLU 159	62.565 13.080 2.721 1.00 22.90
ATOM	22 CG GLU 159	63.847 12.933 1.916 1.00 22.04
ATOM	23 CD GLU 159	64.386 14.260 1.427 1.00 22.07
ATOM	24 OE1 GLU 159	63.577 15.175 1.203 1.00 24.63
ATOM	25 OE2 GLU 159	65.612 14.389 1.240 1.00 23.54
ATOM	26 C GLU 159	61.463 13.717 4.855 1.00 21.56
ATOM	27 O GLU 159	60.747 12.958 5.516 1.00 21.03
ATOM	28 N PRO 160	61.176 15.022 4.713 1.00 19.69
ATOM	29 CD PRO 160	61.997 16.139 4.207 1.00 16.57
ATOM	30 CA PRO 160	59.923 15.500 5.292 1.00 18.12
ATOM	31 CB PRO 160	59.935 16.990 4.955 1.00 15.65
ATOM	32 CG PRO 160	61.390 17.328 4.905 1.00 14.83
ATOM	33 C PRO 160	58.741 14.782 4.626 1.00 19.79
ATOM	34 O PRO 160	58.793 14.431 3.445 1.00 20.20
ATOM	35 N THR 161	57.713 14.497 5.412 1.00 20.15
ATOM	36 CA THR 161	56.525 13.846 4.901 1.00 20.73
ATOM	37 CB THR 161 38 OG1 THR 161	55.672 13.274 6.060 1.00 20.77
ATOM ATOM	38 OG1 THR 161 39 CG2 THR 161	55.195 14.348 6.881 1.00 21.74
ATOM	40 C THR 161	56.489 12.324 6.917 1.00 19.52 55.734 14.054 4.310 1.00 31.64
ATOM	41 O THR 161	55.724 14.954 4.219 1.00 21.64 56.010 16.139 4.421 1.00 23.13
ATOM	42 N PRO 162	54.701 14.596 3.425 1.00 21.21
ATOM	43 CD PRO 162	54.309 13.235 3.012 1.00 19.57
ATOM	44 CA PRO 162	53.884 15.602 2.751 1.00 21.01
ATOM	45 CB PRO 162	52.722 14.776 2.223 1.00 19.74
ATOM	46 CG PRO 162	53.387 13.490 1.861 1.00 20.34
ATOM	47 C PRO 162	53.391 16.643 3.753 1.00 22.52
ATOM	48 O PRO 162	53.508 17.851 3.526 1.00 21.68
ATOM	49 N GLU 163	52.880 16.151 4.878 1.00 23.01
ATOM	•	52.349 16.996 5.941 1.00 25.97
ATOM	51 CB GLU 163	51.672 16.148 7.022 1.00 29.50
	J- 42 420 103	51.5.2 10.110 F.O22 1.00 25.50

52 CG GLU **ATOM** 163 50.476 15.312 6.543 1.00 37.07 **ATOM** 53 CD GLU 163 50.865 14.159 5.614 1.00 41.36 **ATOM** 54 OE1 GLU 163 51.937 13.544 5.828 1.00 40.11 **ATOM** 55 OE2 GLU 163 50.094 13.874 4.660 1.00 46.16 **ATOM** 56 C GLU 163 53.415 17.879 6.581 1.00 24.92 57 O GLU **ATOM** 163 53.110 18.971 7.061 1.00 25.82 **ATOM** 58 N GLU 164 54.661 17.412 6.600 1.00 22,87 **ATOM** 59 CA GLU 164 55.724 18.209 7.187 1.00 21.46 **ATOM** 60 CB GLU 164 56.880 17.340 7.664 1.00 21.23 **ATOM** 61 CG GLU 164 56.509 16.508 8.886 1.00 20.30 **ATOM** 62 CD GLU 164 57.557 15.483 9.243 1.00 20.07 63 OE1 GLU ATOM 164 58.409 15.186 8.385 1.00 19.80 ATOM 64 OE2 GLU 164 57.532 14.977 10.385 1.00 21.00 **ATOM** 65 C GLU 164 6.235 1.00 22.45 56.195 19.289 **ATOM** 66 O **GLU** 164 56.607 20.354 6.684 1.00 23.36 **ATOM** 67 N TRP 165 4.928 1.00 21.06 56.140 19.024 **ATOM** 68 CA TRP 165 56.518 20.031 3.936 1.00 19.57 **ATOM** 69 CB TRP 165 56.486 19.466 2.518 1.00 16.06 70 CG TRP **ATOM** 165 57.775 18.839 2.120 1.00 14.01 **ATOM** 71 CD2 TRP 165 59.055 19.480 2.037 1.00 13.26 **ATOM** 72 CE2 TRP 165 59.976 18.515 1.588 1.00 12.91 **ATOM** 73 CE3 TRP 165 59.507 20.779 2.300 1.00 14.44 **ATOM** 74 CD1 TRP 165 57.972 17.544 1.738 1.00 12.89 **ATOM** 75 NE1 TRP 165 59.290 17.343 1.413 1.00 12.80 **ATOM** 76 CZ2 TRP 165 61.328 18.805 1.388 1.00 15.06 **ATOM** 77 CZ3 TRP 165 60.850 21.069 2.103 1.00 14.72 **ATOM** 78 CH2 TRP 165 61.747 20.084 1.649 1.00 16.82 **ATOM** 79 C TRP 165 55.553 21.210 4.056 1.00 18.93 **ATOM** 80 O TRP 165 55.960 22.359 3.926 1.00 21.12 **ATOM** 81 N **ASP** 166 54.279 20.922 4.307 1.00 19.33 **ATOM** 82 CA ASP 166 53.262 21.963 4.483 1.00 20.35 **ATOM** 83 CB ASP 166 51.864 21.353 4.672 1.00 20.22 51.302 20.748 ATOM 84 CG ASP 166 3.386 1.00 23.36 **ATOM** 85 OD1 ASP 166 51.746 21.153 2.296 1.00 23.42 **ATOM** 86 OD2 ASP 166 50.414 19.878 3.462 1.00 21.02 **ATOM** 87 C ASP 166 53.623 22.785 5.712 1.00 21.02 **ASP** 166 ATOM 88 O 53.627 24.013 5.654 1.00 22.56 **ATOM** 89 N LEU 167 53.926 22.096 6.813 1.00 20.50 90 CA LEU **ATOM** 167 54.312 22.726 8.071 1.00 21.37 **ATOM** 91 CB LEU 167 54.661 21.657 9.109 1.00 23.49 **ATOM** 92 CG LEU 167 54.223 21.846 10.565 1.00 27.19 ATOM 93 CD1 LEU 167 55.312 21.291 11.453 1.00 27.70 **ATOM** 94 CD2 LEU 167 53.940 23.314 10.906 1.00 27.71 **ATOM** 55.541 23.602 7.839 1.00 20.72 95 C LEU 167 **ATOM** 96 O LEU 167 55.601 24.748 8.294 1.00 22.98 **ATOM** 97 N ILE 168 56.505 23.051 7.114 1.00 18.54 **ATOM** 98 CA ILE 168 57.747 23.725 6.778 1.00 18.60

ATOM	. 99 CB ILE 168	58.671 22.771 5.995 1.00 17.54
ATOM	100 CG2 ILE 168	59.695 23.533 5.163 1.00 17.65
ATOM	101 CG1 ILE 168	59.330 21.794 6.972 1.00 20.27
ATOM	102 CD1 ILE 168	60.048 20.631 6.322 1.00 17.96
ATOM	103 C ILE 168	57.486 25.002 5.979 1.00 21.96
ATOM	104 O- ILE 168	58.045 26.064 6.291 1.00 23.06
ATOM	105 N HIS 169	56.591 24.925 4.996 1.00 22.04
ATOM	106 CA HIS 169	56.285 26.092 4.164 1.00 21.21
ATOM	107 CB HIS 169	55.413 25.702 2.969 1.00 20.12
ATOM	108 CG HIS 169	56.101 24.799 2.001 1.00 19.18
ATOM	109 CD2 HIS 169	57.398 24.733 1.619 1.00 18.62
ATOM	110 ND1 HIS 169	55.457 23.764 1.357 1.00 17.90
ATOM	111 CE1 HIS 169	56.327 23.096 0.625 1.00 18.43
ATOM	112 NE2 HIS 169	57.513 23.660 0.772 1.00 20.10
ATOM	113 C HIS 169	55.615 27.198 4.959 1.00 20.61
ATOM	114 O HIS 169	55.979 28.370 4.836 1.00 20.08
ATOM	115 N VAL 170	54.632 26.821 5.769 1.00 20.01
ATOM	116 CA VAL 170	53.922 27.785 6.580 1.00 20.52
ATOM	117 CB VAL 170	52.816 27.120 7.384 1.00 21.33
ATOM	118 CG1 VAL 170	52.224 28.113 8.366 1.00 22.32
ATOM	119 CG2 VAL 170	51.740 26.608 6.438 1.00 23.27
ATOM	120 C VAL 170	54.891 28.477 7.521 1.00 20.58
ATOM	121 O VAL 170	54.926 29.704 7.554 1.00 22.32
ATOM	122 N ALA 171	55.712 27.696 8.230 1.00 18.83
ATOM	123 CA ALA 171	56.692 28.234 9.182 1.00 18.34
ATOM	124 CB ALA 171	57.375 27.102 9.946 1.00 17.05
ATOM	125 C ALA 171	57.733 29.151 8.533 1.00 17.84
ATOM	126 O ALA 171	58.084 30.200 9.091 1.00 18.67
ATOM	127 N THR 172	58.231 28.756 7.367 1.00 17.81
ATOM	128 CA THR 172	59.215 29.551 6.639 1.00 18.88
ATOM	129 CB THR 172	59.726 28.794 5.380 1.00 20.47
ATOM	130 OG1 THR 172	60.280 27.531 5.776 1.00 21.38
ATOM	131 CG2 THR 172	60.806 29.599 4.648 1.00 20.22
ATOM	132 C THR 172	58.655 30.932 6.251 1.00 19.42
ATOM	133 O THR 172	59.320 31.957 6:435 1.00 17.98
ATOM	134 N GLU 173	57.425 30.970 5.756 1.00 19.97
ATOM	135 CA GLU 173	56.811 32.236 5.374 1.00 22.51
ATOM	136 CB GLU 173	55.520 31.981 4.577 1.00 27.26
ATOM ATOM	137 CG GLU 173 138 CD GLU 173	54.823 33.244 4.005 1.00 34.96
		55.690 34.040 3.020 1.00 39.54
ATOM ATOM	139 OE1 GLU 173 140 OE2 GLU 173	56.610 33.454 2.395 1.00 41.82
ATOM	·	55.443 35.259 2.872 1.00 41.06
ATOM		56.538 33.099 6.622 1.00 21.60 56.736 34.313 6.505 1.00 21.73
ATOM		56.726 34.313 6.595 1.00 21.73
ATOM	143 N ALA 174 144 CA ALA 174	56.123 32.461 7.716 1.00 19.69
ATOM	145 CB ALA 174	55.844 33.155 8.968 1.00 18.07 55.423 32.169 10.037 1.00 16.90
1110141	140 CD ALA 1/4	33. 723 32.103 10.03/ 1.00 10.90

ATOM .146 C **ALA** 174 57.101 33.883 9.400 1.00 17.65 **ATOM** 147 O **ALA** 174 57.052 35.031 9.829 1.00 19.80 **ATOM** 148 N HIS 175 58.240 33.222 9.259 1.00 16.39 **ATOM** 149 CA HIS 175 59.498 33.831 9.629 1.00 16.41 **ATOM** 150 CB HIS 175 60.574 32.758 9.804 1.00 12.71 **ATOM** 151 CG HIS 175 61.938 33.318 10.043 1.00 11.09 **ATOM** 152 CD2 HIS 175 62.373 34.252 10.920 1.00 8.26 **ATOM** 153 ND1 HIS 175 63.030 32.977 9.273 1.00 13.39 ATOM 154 CE1 HIS 175 64.076 33.683 9.658 1.00 13.77 155 NE2 HIS **ATOM** 175 63.702 34.464 10.658 1.00 12.70 **ATOM** 156 C HIS 175 59.959 34.903 8.624 1.00 19.55 **ATOM** HIS 157 O 175 60.293 36.027 9.016 1.00 18.38 **ATOM** 158 N **ARG** 176 59.987 34.555 7.339 1.00 20.77 **ATOM 159 CA ARG** 176 60.424 35.494 6.307 1.00 21.30 160 CB ARG **ATOM** 176 60.315 34.876 4.917 1.00 24.87 **ATOM** 161 CG ARG 176 61.361 33.827 4.609 1.00 30.22 **ATOM** 162 CD ARG 176 61.429 33.603 3.116 1.00 36.29 **ATOM 163 NE ARG** 176 62.256 32.457 2.758 1.00 44.72 **ATOM** 164 CZ ARG 176 62.031 31.680 1.700 1.00 49.80 **ATOM** 165 NH1 ARG 176 61.000 31.935 0.894 1.00 50.83 **ATOM** 166 NH2 ARG 176 62.812 30.627 1.466 1.00 50.14 **ATOM** 167 C **ARG** 176 59.658 36.807 6.337 1.00 20.67 **ATOM** 168 O ARG 176 60.256 37.877 6.238 1.00 20.53 **ATOM** 169 N SER 177 58.344 36.730 6.508 1.00 20.67 **ATOM** 57.526 37.934 6.551 1.00 21.86 170 CA SER 177 **ATOM** 171 CB SER 177 56.061 37.588 6.298 1.00 19.59 **ATOM** 172 OG SER 177 55.541 36.774 7.329 1.00 21.85 **ATOM** 173 C SER 177 57.659 38.733 7.857 1.00 23.27 **ATOM** 174 O SER 177 57.073 39.807 7.989 1.00 24.40 175 N **ATOM** THR 178 58.383 38.202 8.837 1.00 22.16 **ATOM** 176 CA THR 178 58.542 38.913 10.095 1.00 20.62 **ATOM** 177 CB THR 178 57.853 38.162 11.265 1.00 19.93 **ATOM** 178 OG1 THR 178 58.386 36.838 11.381 1.00 18.72 **ATOM** 179 CG2 THR 178 56.359 38.057 11.033 1.00 16.95 **ATOM** 180 C THR 178 60.015 39.137 10:394 1.00 21.57 **ATOM** 181 O THR 178 60.368 39.649 11.449 1.00 23.91 182 N ASN 179 **ATOM** 60.870 38.769 9.445 1.00 22.22 **ATOM 183 CA ASN** 179 62.316 38.912 9.585 1.00 24.22 **ATOM 184 CB ASN** 179 63.013 37.690 8.970 1.00 22.49 **ATOM 185 CG ASN** 179 64.480 37.596 9.344 1.00 23.53 **ATOM** 186 OD1 ASN 179 64.866 37.912 10.464 1.00 22.32 **ATOM** 187 ND2 ASN 179 65.296 37.100 8.425 1.00 23.84 **ATOM** 188 C ASN 179 62.744 40.210 8.881 1.00 26.52 **ATOM** 189 O **ASN** 179 62.923 40.253 7.657 1.00 26.65 **ATOM** 190 N ALA 180 9.671 1.00 27.47 62.898 41.267 **ATOM** 191 CA ALA 180 63.255 42.582 9.166 1.00 30.30 **ATOM** 192 CB ALA 180 63.552 43.508 10.321 1.00 27.21

ATOM	193 C ALA 180	64.404 42.593 8.166 1.00 33.14
ATOM	194 O ALA 180	65.440 41.972 8.397 1.00 33.71
ATOM	195 N GLN 181	64.209 43.295 7.049 0.50 35.09
ATOM	196 CA GLN 181	65.212 43.423 5.980 0.50 37.44
ATOM	197 CB GLN 181	66.544 43.974 6.511 0.50 38.60
ATOM	198 CG GLN 181	66.728 45.462 6.299 0.50 40.53
ATOM	199 CD GLN 181	65.805 46.291 7.162 0.50 42.72
ATOM	200 OE1 GLN 181	64.639 46.512 6.828 0.50 42.05
ATOM	201 NE2 GLN 181	66.324 46.756 8.284 0.50 44.59
ATOM	202 C GLN 181	65.481 42.180 5.138 0.50 38.43
ATOM	203 O GLN 181	66.175 42.262 4.118 0.50 38.92
ATOM	204 N GLY 182	64.958 41.034 5.562 1.00 38.74
ATOM	205 CA GLY 182	65.166 39.808 4.805 1.00 40.07
ATOM	206 C GLY 182	66.634 39.554 4.486 1.00 42.06
ATOM	207 O GLY 182	67.504 39.684 5.346 1.00 43.28
ATOM	208 N SER 183	66.926 39.272 3.224 1.00 43.72
ATOM	209 CA SER 183	68.299 39.001 2.812 1.00 45.88
ATOM	210 CB SER 183	68.304 38.069 1.593 1.00 47.26
ATOM	211 OG SER 183	67.519 38.605 0.531 1.00 47.23
ATOM	212 C SER 183	69.095 40.268 2.497 1.00 46.24
ATOM	213 O SER 183	70.290 40.194 2.185 1.00 48.13
ATOM	214 N HIS 184	68.445 41.426 2.579 1.00 45.79
ATOM	215 CA HIS 184	69.111 42.690 2.276 1.00 45.00
ATOM	216 CB HIS 184	68.127 43.636 1.594 1.00 43.54
ATOM ATOM	217 C HIS 184 218 O HIS 184	69.732 43.351 3.516 1.00 44.67
ATOM	218 O HIS 184 219 N TRP 185	70.316 44.440 3.428 1.00 45.02 69.659 42.663 4.653 1.00 43.24
ATOM	220 CA TRP 185	69.659 42.663 4.653 1.00 43.24 70.190 43.172 5.919 1.00 40.98
ATOM	221 CB TRP 185	70.190 43.172 3.919 1.00 40.98
ATOM	222 CG TRP 185	70.889 40.874 6.775 1.00 34.14
ATOM	223 CD2 TRP 185	72.197 40.593 7.291 1.00 33.38
ATOM	224 CE2 TRP 185	72.572 39.321 6.807 1.00 31.68
ATOM	225 CE3 TRP 185	73.092 41.296 8.107 1.00 31.65
ATOM	226 CD1 TRP 185	70.530 39.790 6.028 1.00 34.27
ATOM	227 NE1 TRP 185	71.536 38.852 6.043 1.00 33.51
ATOM .	228 CZ2 TRP 185	73.795 38.733 7.121 1.00 31.67
ATOM	229 CZ3 TRP 185	74.308 40.713 8.419 1.00 31.29
ATOM	230 CH2 TRP 185	74.651 39.444 7.923 1.00 31.06
ATOM	231 C TRP 185	71.618 43.720 5.856 1.00 41.52
ATOM	232 O TRP 185	71.893 44.817 6.335 1.00 40.52
ATOM	233 N LYS 186	72.520 42.976 5.234 1.00 42.94
ATOM	234 CA LYS 186	73.896 43.417 5.143 1.00 45.25
ATOM	235 CB LYS 186	74.764 42.328 4.508 1.00 45.96
ATOM	236 CG LYS 186	76.255 42.600 4.590 1.00 48.07
ATOM	237 CD LYS 186	77.053 41.307 4.504 1.00 51.20
ATOM	238 CE LYS 186	78.554 41.574 4.457 1.00 52.69
ATOM	239 NZ LYS 186	78.975 42.277 3.201 1.00 55.56

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ATOM	240 C LYS 186	74.025 44.730 4.377 1.00 47.38
ATOM	241 O LYS 186	74.914 45.535 4.663 1.00 47.65
ATOM	242 N GLN 187	73.134 44.959 3.418 0.50 48.02
ATOM	243 CA GLN 187	73.193 46.183 2.623 0.50 48.69
ATOM	244 CB GLN 187	72.547 45.973 1.246 0.50 48.66
ATOM	245 CG GLN 187	73.104 44.771 0.453 0.50 49.05
ATOM	246 CD GLN 187	74.624 44.766 0.339 0.50 49.17
ATOM	247 OE1 GLN 187	75.225 45.691 -0.209 0.50 49.71
ATOM	248 NE2 GLN 187	75.250 43.710 0.847 0.50 48.57
ATOM	249 C GLN 187	72.551 47.373 3.343 0.50 49.06
ATOM	250 O GLN 187	73.094 48.475 3.329 0.50 49.53
ATOM	251 N ARG 188	71.405 47.152 3.980 1.00 49.18
ATOM	252 CA ARG 188	70.723 48.221 4.695 1.00 49.90
ATOM	253 CB ARG 188	69.209 47.988 4.653 1.00 53.68
ATOM	254 CG ARG 188	68.617 47.798 3.251 1.00 57.22
ATOM	255 CD ARG 188	67.099 47.962 3.302 1.00 60.67
ATOM	256 NE ARG 188	66.430 47.441 2.110 1.00 64.43
ATOM	257 CZ ARG 188	65.931 46.208 2.009 1.00 66.13
ATOM	258 NH1 ARG 188	66.027 45.362 3.031 1.00 66.69
ATOM	259 NH2 ARG 188	65.318 45.823 0.893 1.00 66.10
ATOM	260 C ARG 188	71.150 48.510 6.133 1.00 48.42
ATOM	261 O ARG 188	70.544 49.368 6.784 1.00 48.86
ATOM	262 N ARG 189	72.153 47.804 6.647 1.00 46.00
ATOM	263 CA ARG 189	72.581 48.030 8.028 1.00 44.24
ATOM ATOM	264 CB ARG 189	73.039 46.726 8.690 1.00 43.40
ATOM	265 CG ARG 189 266 CD ARG 189	74.367 46.204 8.203 1.00 43.05
ATOM	267 NE ARG 189	74.808 45.021 9.019 1.00 43.62 76.185 44.660 8.717 1.00 45.95
ATOM	268 CZ ARG 189	76.185 44.660 8.717 1.00 45.95 76.981 43.976 9.536 1.00 48.56
ATOM	269 NH1 ARG 189	76.548 43.560 10.724 1.00 46.34
ATOM	270 NH2 ARG 189	78.233 43.735 9.174 1.00 40.34 78.239 73.735 73.74 73.75 73.
ATOM	271 C ARG 189	73.642 49.116 8.238 1.00 43.20
ATOM	272 O ARG 189	74.629 49.210 7.500 1.00 43.07
ATOM	273 N LYS 190	73.427 49.925 9.268 1.00 41.56
ATOM	274 CA LYS 190	74.335 51.003 9.628 1.00 39.96
ATOM	275 CB LYS 190	73.563 52.323 9.757 1.00 38.85
ATOM	276 C LYS 190	74.983 50.631 10.956 1.00 38.91
ATOM	277 O LYS 190	74.345 50.015 11.806 1.00 38.17
ATOM	278 N PHE 191	76.261 50.959 11.104 1.00 38.49
ATOM	279 CA PHE 191	76.998 50.673 12.326 1.00 38.42
ATOM	280 CB PHE 191	78.500 50.762 12.073 1.00 38.37
ATOM	281 CG PHE 191	79.056 49.608 11.308 1.00 39.05
ATOM	282 CD1 PHE 191	78.712 49.408 9.976 1.00 40.02
ATOM	283 CD2 PHE 191	79.942 48.727 11.917 1.00 39.19
ATOM	284 CE1 PHE 191	79.245 48.344 9.256 1.00 40.57
ATOM	285 CE2 PHE 191	80.482 47.661 11.213 1.00 40.32
ATOM	286 CZ PHE 191	80.133 47.466 9.875 1.00 41.84

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ATOM .287 C PHE 191 76.650 51.673 13.416 1.00 37.96 **ATOM** 288 O PHE 191 76.568 52.872 13.151 1.00 38.95 **ATOM** 289 N LEU 192 76.433 51.184 14.634 1.00 37.05 **ATOM** 290 CA LEU 192 76.138 52.063 15.759 1.00 35.99 **ATOM** 291 CB LEU 192 75.833 51.247 17.014 1.00 33.04 **ATOM** 292 CG LEU 192 75.503 52.074 18.260 1.00 31.38 **ATOM** 293 CD1 LEU 192 74.116 52.651 18.102 1.00 29.02 **ATOM** 294 CD2 LEU 192 75.592 51.229 19.536 1.00 30.32 **ATOM** 295 C LEU 192 77.436 52.831 15.976 1.00 36.99 **ATOM** 296 O LEU 192 78.500 52.218 16.112 1.00 37.66 **ATOM** 297 N PRO 193 77.377 54.177 15.988 1.00 38.15 **ATOM** 298 CD PRO 193 76.156 54.996 15.902 1.00 37.90 **ATOM** 299 CA PRO 193 78.561 55.025 16.187 1.00 38.68 **ATOM** 300 CB PRO 193 77.950 56.365 16.568 1.00 37.20 **ATOM** 301 CG PRO 193 76.711 56.397 15.758 1.00 37.08 **ATOM** 302 C PRO 193 79.475 54.503 17.294 1.00 41.12 **ATOM** 303 O **PRO** 193 79.005 54.129 18.367 1.00 42.26 ATOM 304 N **ASP** 194 80.782 54.509 17.052 1.00 43.62 **ATOM** 305 CA ASP 194 81.731 54.012 18.050 1.00 46.71 **ATOM** 306 CB ASP 194 83.131 53.938 17.470 1.00 49.32 **ATOM** 307 CG ASP 194 83.237 52.904 16.397 1.00 52.34 **ATOM** 308 OD1 ASP 194 83.539 51.726 16.719 1.00 53.18 **ATOM** 309 OD2 ASP 194 82.981 53.268 15.227 1.00 55.10 **ATOM** 310 C **ASP** 194 81.769 54.743 19.386 1.00 47.12 **ATOM ASP** 311 O 194 82.158 54.163 20.403 1.00 48.16 **ATOM** 312 N ASP 195 81.389 56.015 19.386 1.00 47.54 **ATOM 313 CA ASP** 195 81.382 56.791 20.620 1.00 48.68 **ATOM** 314 CB ASP 195 81.180 58.285 20.322 1.00 50.76 **ATOM** 315 CG ASP 195 79.871 58.572 19.602 1.00 54.24 **ATOM** 316 OD1 ASP 195 78.929 59.082 20.253 1.00 56.17 **ATOM** 317 OD2 ASP 79.786 58.292 18.385 1.00 56.08 195 **ATOM ASP** 318 C 195 80.304 56.274 21.580 1.00 47.63 **ATOM ASP** 319 O 195 80.294 56.621 22.772 1.00 49.07 **ATOM** 320 N ILE 196 79.400 55.444 21.065 1.00 44.87 **ATOM 321 CA ILE** 196 78.330 54.890 21:888 1.00 42.53 **ATOM** 322 CB ILE 196 76.983 54.813 21.121 1.00 42.19 **ATOM** 323 CG2 ILE 196 75.870 54.357 22.060 1.00 40.29 **ATOM** 324 CG1 ILE 196 76.635 56.191 20.535 1.00 41.32 **ATOM** 325 CD1 ILE 196 75.344 56.219 19.732 1.00 41.32 **ATOM** 326 C ILE 78.725 53.509 22.391 1.00 40.89 196 **ATOM** 327 O ILE 196 79.358 52.722 21.679 1.00 40.08 **ATOM** 328 N GLY 197 78.384 53.240 23.642 1.00 40.16 **ATOM** 329 CA GLY 197 78.705 51.957 24.228 1.00 40.21 **ATOM** 330 C **GLY** 197 80.066 51.907 24.879 1.00 40.18 **ATOM** 331 O **GLY** 197 80.512 50.839 25.267 1.00 40.55 80.718 53.057 25.029 1.00 41.25 **ATOM** 332 N GLN 198 **ATOM** 333 CA GLN 198 82.038 53.111 25.664 1.00 40.94

ATOM	334 CB GLN 198	83.041 53.823 24.738 1.00 39.51
ATOM	335 C GLN 198	81.995 53.796 27.046 1.00 40.93
ATOM	336 O GLN 198	83.036 54.197 27.571 1.00 41.83
ATOM	337 N SER 199	80.806 53.859 27.654 1.00 39.68
ATOM	338 CA SER 199	80.615 54.510 28.961 1.00 37.74
ATOM	339 CB SER 199	79.995 55.905 28.768 1.00 38.50
ATOM	340 OG SER 199	80.687 56.672 27.792 1.00 40.71
ATOM	341 C SER 199	79.743 53.726 29.958 1.00 36.31
ATOM	342 O SER 199	78.719 54.228 30.436 1.00 35.69
ATOM	343 N PRO 200	80.123 52.484 30.280 1.00 35.05
ATOM	344 CD PRO 200	81.246 51.684 29.760 1.00 33.97
ATOM	345 CA PRO 200	79.313 51.715 31.228 1.00 35.89
ATOM	346 CB PRO 200	79.872 50.304 31.075 1.00 33.94
ATOM	347 CG PRO 200	81.297 50.532 30.708 1.00 33.31
ATOM	348 C PRO 200	79.477 52.241 32.656 1.00 37.75
ATOM	349 O PRO 200	80.484 51.959 33.299 1.00 38.78
ATOM	350 N ILE 201	78.493 52.988 33.158 1.00 39.61
ATOM	351 CA ILE 201	78.590 53.551 34.511 1.00 40.56
ATOM	352 CB ILE 201	78.715 55.093 34.484 1.00 40.20
ATOM	353 CG2 ILE 201	80.125 55.501 34.082 1.00 41.06
ATOM	354 CG1 ILE 201	77.690 55.694 33.532 1.00 40.98
ATOM	355 CD1 ILE 201	77.969 57.147 33.205 1.00 44.31
ATOM	356 C ILE 201	77.535 53.160 35.546 1.00 41.40
ATOM	357 O ILE 201	77.768 53.313 36.751 1.00 42.09
ATOM	358 N VAL 202	76.365 52.701 35.104 1.00 41.42
ATOM	359 CA VAL 202	75.325 52.293 36.053 1.00 40.70
ATOM	360 CB VAL 202	73.913 52.292 35.422 1.00 38.44
ATOM	361 CG1 VAL 202	72.881 51.826 36.435 1.00 35.91
ATOM	362 CG2 VAL 202	73.560 53.692 34.934 1.00 36.42
ATOM	363 C VAL 202	75.687 50.917 36.622 1.00 41.64
ATOM	364 O VAL 202	76.094 50.008 35.894 1.00 42.05
ATOM	365 N SER 203	75.596 50.800 37.938 1.00 43.06
ATOM	366 CA SER 203	75.947 49.576 38.639 1.00 44.57
ATOM	367 CB SER 203	75.916 49.842 40.154 1.00 46.82
ATOM	368 OG SER 203	76.457 48.772 40.916 1.00 50.18
ATOM	369 C SER 203	75.052 48.388 38.294 1.00 44.08
ATOM	370 O SER 203	73.849 48.534 38.093 1.00 44.28
ATOM	371 N MET 204	75.656 47.210 38.231 1.00 43.11
ATOM	372 CA MET 204	74.930 45.980 37.963 1.00 43.12
ATOM	373 CB MET 204	75.048 45.557 36.494 1.00 41.07
ATOM	374 CG MET 204	74.126 46.320 35.554 1.00 36.96
ATOM	375 SD MET 204	72.375 46.134 35.990 1.00 38.66
ATOM	376 CE MET 204	71.970 44.592 35.098 1.00 37.26
ATOM	377 C MET 204	75.561 44.943 38.866 1.00 43.68
ATOM	378 O MET 204	76.784 44.817 38.912 1.00 44.32
ATOM	379 N PRO 205	74.735 44.204 39.619 1.00 44.22
ATOM	380 CD PRO 205	73.261 44.310 39.610 1.00 44.44

ATOM .381 CA PRO 205 75.187 43.164 40.546 1.00 44.32 **ATOM** 382 CB PRO 205 73.944 42.299 40.701 1.00 45.18 **ATOM** 383 CG PRO 205 72.832 43.335 40.691 1.00 44.29 **ATOM** 384 C PRO 205 76.417 42.354 40.122 1.00 44.31 **ATOM** 385 O **PRO** 205 77.393 42.293 40.864 1.00 43.97 **ATOM** 386 N. ASP 206 76.404 41.802 38.912 1.00 44.30 **ATOM** 387 CA ASP 206 77.524 40.984 38.433 1.00 44.77 **ATOM** 388 CB ASP 206 77.073 40.106 37.270 1.00 47.12 **ATOM 389 CG ASP** 206 76.503 40.912 36.120 1.00 49.73 **ATOM** 390 OD1 ASP 206 76.992 42.039 35.863 1.00 49.65 **ATOM** 391 OD2 ASP 206 75.553 40.416 35.478 1.00 51.96 **ATOM** 392 C **ASP** 206 78.805 41.718 38.037 1.00 44.10 **ATOM** 393 O **ASP** 206 79.754 41.099 37.549 1.00 43.60 **ATOM** 394 N GLY 207 78.804 43.039 38.145 1.00 44.19 **ATOM** 395 CA GLY 207 80.001 43.785 37.803 1.00 43.51 **ATOM** 396 C GLY 207 80.041 44.425 36.433 1.00 43.29 **ATOM** 397 O **GLY** 207 80.745 45.421 36.257 1.00 44.47 **ATOM ASP** 79.363 43.845 35.446 1.00 42.45 398 N 208 **ATOM** 399 CA ASP 208 79.347 44.436 34.106 1.00 41.51 **ATOM** 400 CB ASP 208 78.915 43.402 33.070 1.00 42.91 **ATOM** 401 CG ASP 208 80.001 42.379 32.785 1.00 43.57 **ATOM** 402 OD1 ASP 208 79.675 41.218 32.468 1.00 44.55 **ATOM** 403 OD2 ASP 208 81.191 42.742 32.868 1.00 47.14 **ASP** ATOM 404 C 208 78.378 45.606 34.143 1.00 40.78 **ATOM** 405 O ASP 208 77.176 45.403 34.277 1.00 42.50 **ATOM** 406 N LYS 209 78.902 46.827 34.058 1.00 39.10 **ATOM** 407 CA LYS 209 78.071 48.033 34.150 1.00 37.23 **ATOM** 408 CB LYS 78.910 49.211 34.681 1.00 37.29 209 **ATOM** 409 C LYS 209 77.326 48.423 32.871 1.00 34.47 **ATOM** 410 O LYS 209 77.707 48.013 31.776 1.00 33.85 **ATOM** 411 N VAL 210 76.275 49.228 33.028 1.00 33.30 **ATOM** 412 CA VAL 210 75.448 49.684 31.907 1.00 31.78 **ATOM** 413 CB VAL 210 73.929 49.618 32.235 1.00 29.51 **ATOM** 414 CG1 VAL 210 73.102 50.012 31.010 1.00 29.24 **ATOM** 415 CG2 VAL 210 73.541 48.237 32.698 1.00 29.84 **ATOM** 416 C VAL 210 75.731 51.115 31.451 1.00 32.68 **ATOM** 417 O VAL 210 75.845 52.033 32.264 1.00 32.69 418 N **ATOM** ASP 211 75.769 51.290 30.134 1.00 33.00 **ATOM** 419 CA ASP 211 75.978 52.574 29.476 1.00 31.85 **ATOM** 420 CB ASP 211 76.826 52.353 28.221 1.00 32.38 **ATOM** 421 CG ASP 211 77.019 53.612 27.386 1.00 31.88 **ATOM** 422 OD1 ASP 211 78.123 53.768 26.843 1.00 32.78 **ATOM** 423 OD2 ASP 211 76.079 54.412 27.208 1.00 32.32 **ATOM** 424 C **ASP** 74.562 53.023 29.101 1.00 33.39 211 **ATOM** 425 O **ASP** 211 73.925 52.444 28.206 1.00 31.94 **ATOM** 426 N LEU 212 74.078 54.063 29.770 1.00 32.50 **ATOM** 427 CA LEU 212 72.731 54.568 29.532 1.00 32.29

ATOM .428 CB LEU 212 72.440 55.736 30.470 1.00 32.41 **ATOM** 429 CG LEU 212 72.311 55.336 31.936 1.00 32.11 **ATOM** 430 CD1 LEU 212 72.447 56.555 32.830 1.00 32.35 **ATOM** 431 CD2 LEU 212 70.979 54.650 32.148 1.00 30.87 **ATOM** 432 C LEU 212 72.419 54.962 28.092 1.00 32.29 **ATOM** 433 O- LEU 212 71.326 54.695 27.609 1.00 32.13 **ATOM** 434 N GLU 213 73.370 55.589 27.407 1.00 32.21 73.144 56.007 26.028 1.00 33.12 ATOM 435 CA GLU 213 **ATOM** 436 CB GLU 213 74.305 56.864 25.530 1.00 36.72 **ATOM** 437 CG GLU 213 74.067 57.468 24.146 1.00 40.61 **ATOM** 438 CD GLU 213 75.316 58.101 23.545 1.00 44.21 **ATOM** 439 OE1 GLU 213 76.434 57.851 24.059 1.00 46.23 **ATOM** 440 OE2 GLU 213 75.178 58.836 22.543 1.00 45.81 **ATOM** 441 C GLU 213 72.966 54.801 25.111 1.00 31.91 **ATOM** 442. O GLU 213 72.064 54.775 24.273 1.00 31.31 ATOM 443 N ALA 214 73.827 53.803 25.285 1.00 30.66 **ATOM** 444 CA ALA 214 73.769 52.585 24.482 1.00 30.43 **ATOM** 445 CB ALA 214 74.971 51.690 24.783 1.00 29.77 **ATOM** 446 C ALA 214 72.464 51.854 24.778 1.00 29.34 **ATOM** 447 O ALA 214 71.772 51.421 23.862 1.00 28.33 **ATOM** 448 N PHE 215 72.116 51.762 26.058 1.00 28.45 **ATOM** 449 CA PHE 215 70.882 51.116 26.492 1.00 29.05 **ATOM** 450 CB PHE 215 70.732 51.240 28.005 1.00 25.98 **ATOM** 69.443 50.689 28.535 1.00 25.53 451 CG PHE 215 **ATOM** 452 CD1 PHE 215 69.330 49.344 28.854 1.00 26.16 **ATOM** 453 CD2 PHE 215 68.349 51.519 28.737 1.00 25.04 **ATOM** 454 CE1 PHE 215 68.144 48.831 29.370 1.00 25.73 **ATOM** 455 CE2 PHE 215 67.160 51.018 29.252 1.00 25.84 456 CZ PHE **ATOM** 215 67.058 49.669 29.570 1.00 25.25 **ATOM** 457 C PHE 215 69.694 51.780 25.801 1.00 30.92 **ATOM** 458 O PHE 215 68.773 51.107 25.316 1.00 30.38 **ATOM** 459 N SER 216 69.714 53.108 25.776 1.00 31.41 **ATOM** 460 CA SER 216 68.667 53.887 25.136 1.00 31.23 **ATOM** 461 CB SER 216 68.976 55.375 25.256 1.00 32.50 **ATOM** 462 OG SER 216 67.972 56.153 24.628 1.00 35.83 **ATOM** 463 C SER 216 68.600 53.504 23.663 1.00 31.67 **ATOM** 464 O SER 216 67.527 53.235 23.129 1.00 31.34 **ATOM** 465 N GLU 217 69.756 53.475 23.014 1.00 31.72 **ATOM** 466 CA GLU 217 69.823 53.121 21.609 1.00 33.06 **ATOM** 467 CB GLU 217 71.269 53.153 21.110 1.00 34.93 71.824 54.557 20.921 1.00 38.98 ATOM 468 CG GLU 217 469 CD GLU **ATOM** 217 70.986 55.399 19.963 1.00 41.92 **ATOM** 470 OE1 GLU 217 70.177 56.221 20.444 1.00 44.02 **ATOM** 471 OE2 GLU 217 71.139 55.246 18.731 1.00 44.46 **ATOM** 472 C GLU 217 69.199 51.759 21.330 1.00 31.78 **ATOM** 473 O **GLU** 217 68.447 51.607 20.369 1.00 32.51 **ATOM** 474 N PHE 218 69.477 50.779 22.181 1.00 29.80

ATOM	475 CA PHE 218	68.924 49.447 21.979 1.00 27.65
ATOM	476 CB PHE 218	69.668 48.416 22.827 1.00 26.79
ATOM	477 CG PHE 218	71.114 48.292 22.467 1.00 24.76
ATOM	478 CD1 PHE 218	72.083 48.191 23.446 1.00 24.37
ATOM	479 CD2 PHE 218	71.510 48.354 21.134 1.00 24.30
ATOM	480 CE1 PHE 218	73.424 48.167 23.106 1.00 23.85
ATOM	481 CE2 PHE 218	72.843 48.329 20.785 1.00 23.07
ATOM	482 CZ PHE 218	73.804 48.236 21.772 1.00 24.45
ATOM	483 C PHE 218	67.441 49.403 22.255 1.00 26.94
ATOM	484 O PHE 218	66.658 48.985 21.409 1.00 27.98
ATOM	485 N THR 219	67.032 49.906 23.405 1.00 26.97
ATOM	486 CA THR 219	65.619 49.876 23.740 1.00 27.25
ATOM	487 CB THR 219	65.379 50.304 25.195 1.00 27.35
ATOM	488 OG1 THR 219	65.924 51.612 25.410 1.00 26.48
ATOM	489 CG2 THR 219	66.034 49.303 26.139 1.00 24.51
ATOM	490 C THR 219	64.747 50.689 22.782 1.00 27.21
ATOM	491 O THR 219	63.588 50.348 22.557 1.00 28.58
ATOM	492 N LYS 220	65.318 51.726 22.184 1.00 26.75
ATOM	493 CA LYS 220	64.576 52.569 21.254 1.00 27.81
ATOM	494 CB LYS 220	65.439 53.753 20.782 1.00 27.46
ATOM	495 C LYS 220	64.058 51.772 20.056 1.00 28.62
ATOM	496 O LYS 220	63.014 52.101 19.500 1.00 28.63
ATOM	497 N ILE 221	64.774 50.721 19.662 1.00 28.92
ATOM	498 CA ILE 221	64.331 49.907 18.527 1.00 28.19
ATOM	499 CB ILE 221	65.450 49.732 17.465 1.00 27.17
ATOM	500 CG2 ILE 221	65.866 51.095 16.911 1.00 26.61
ATOM	501 CG1 ILE 221	66.645 48.977 18.061 1.00 26.80
ATOM	502 CD1 ILE 221	67.621 48.417 17.029 1.00 24.91
ATOM	503 C ILE 221	63.840 48.512 18.937 1.00 28.82
ATOM	504 O ILE 221	63.552 47.678 18.076 1.00 28.59
ATOM	505 N ILE 222	63.690 48.263 20.236 1.00 27.09
ATOM	506 CA ILE 222	63.279 46.934 20.665 1.00 27.22
ATOM		63.777 46.591 22.101 1.00 26.58
ATOM		62.815 47.151 23.171 1.00 23.83
ATOM		63.949 45.065 22.230 1.00 24.15
ATOM		64.727 44.610 23.458 1.00 21.43
ATOM		61.797 46.614 20.519 1.00 28.33
	512 O ILE 222	
		60.929 47.618 20.622 1.00 27.63
	514 CA THR 223	
ATOM	515 CB THR 223	
ATOM	516 OG1 THR 223	58.839 48.983 22.180 1.00 30.67
ATOM.	517 CG2 THR 223	57.183 48.390 20.525 1.00 26.50
	518 C THR 223	
	519 O THR 223	58.390 45.691 19.196 1.00 24.87
ATOM	520 N PRO 224	
ATOM	521 CD PRO 224	60.138 48.580 17.792 1.00 22.28

ATOM 522 CA PRO 224 59.181 46.612 16.759 1.00 23.13 **ATOM** 523 CB PRO 224 59.747 47.570 15.699 1.00 22.96 **ATOM** 524 CG PRO 224 60.762 48.406 16.443 1.00 24.53 **ATOM** 525 C PRO 224 59.790 45.204 16.634 1.00 22.56 **ATOM** 526 O PRO 224 59.198 44.332 15.994 1.00 22.77 **ATOM** 527 N. ALA 225 60.960 44.989 17.240 1.00 19.17 **ATOM** 528 CA ALA 225 61.622 43.684 17.213 1.00 18.54 **ATOM** 529 CB ALA 225 63.009 43.773 17.806 1.00 16.79 **ATOM** 530 C ALA 225 60.802 42.643 17.969 1.00 19.08 **ATOM** 531 O ALA 225 60.681 41.502 17.523 1.00 21.30 **ATOM** 532 N ILE 226 60.253 43.033 19.117 1.00 18.30 **ATOM** 533 CA ILE 226 59.420 42.147 19.929 1.00 18.65 **ATOM** 534 CB ILE 226 59.092 42.779 21.288 1.00 17.30 **ATOM** 535 CG2 ILE 226 58.057 41.952 22.020 1.00 17.76 **ATOM** 536 CG1 ILE 226 60.361 42.915 22.123 1.00 17.07 **ATOM** 537 CD1 ILE 226 60.175 43.775 23.351 1.00 14.65 **ATOM** 538 C ILE 226 58.109 41.858 19.199 1.00 19.56 **ATOM** 539 O ILE 226 57.638 40.719 19.163 1.00 19.51 540 N **ATOM** THR 227 57.521 42.903 18.627 1.00 20.26 227 **ATOM** 541 CA THR 56.278 42.782 17.881 1.00 21.19 **ATOM** 542 CB THR 227 55.856 44.150 17.326 1.00 22.41 **ATOM** 543 OG1 THR 227 55.670 45.053 18.420 1.00 25.09 227 **ATOM** 544 CG2 THR 54.558 44.041 16.560 1.00 24.29 **ATOM** 545 C THR 227 56.411 41.758 16.742 1.00 20.16 ATOM 546 O THR 227 55.487 40.978 16.496 1.00 21.18 228 **ATOM** 547 N **ARG** 57.558 41.744 16.069 1.00 18.42 **ATOM** 548 CA ARG 228 57.783 40.786 14.991 1.00 18.29 **ATOM** 549 CB ARG 228 59.032 41.136 14.191 1.00 19.95 **ATOM** 550 CG ARG 228 58.810 42.349 13.286 1.00 23.31 **ATOM** 551 CD ARG 228 60.001 42.646 12.405 1.00 25.64 ATOM 552 NE ARG 228 61.139 43.138 13.171 1.00 27.01 **ATOM** 553 CZ ARG 228 62.209 42.413 13.468 1.00 28.20 **ATOM** 554 NH1 ARG 228 62.280 41.155 13.067 1.00 28.99 **ATOM** 555 NH2 ARG 228 63.219 42.951 14.141 1.00 27.25 **ATOM** 556 C ARG 228 57.834 39.352 15.502 1.00 18.40 **ATOM** 557 O ARG 228 57.433 38.431 14.788 1.00 17.50 **ATOM** 558 N VAL 229 58.278 39.162 16.747 1.00 17.42 **ATOM** 559 CA VAL 229 58.316 37.822 17.334 1.00 16.40 229 59.116 37.779 18.674 1.00 15.88 **ATOM** 560 CB VAL 229 **ATOM** 561 CG1 VAL 58.955 36.422 19.334 1.00 16.19 **ATOM** 562 CG2 VAL 229 60.591 38.010 18.421 1.00 14.44 **ATOM** 229 563 C VAL 56.852 37.408 17.552 1.00 16.75 **ATOM** 564 O VAL 229 56.456 36.282 17.219 1.00 16.06 **ATOM** 565 N VAL 230 56.039 38.343 18.046 1.00 16.09 **ATOM** 566 CA VAL 230 54.612 38.097 18.266 1.00 16.97 **ATOM** 567 CB VAL 230 53.896 39.327 18.897 1.00 18.60 **ATOM** 568 CG1 VAL 230 52.401 39.084 18.972 1.00 17.19

ATOM 569 CG2 VAL 230 54.445 39.629 20.299 1.00 17.82 **ATOM** 570 C VAL 230 53.938 37.780 16.916 1.00 18.46 **ATOM** 571 O VAL 230 53.115 36.863 16.828 1.00 18.46 **ATOM** 572 N **ASP** 231 54.289 38.539 15.874 1.00 19.21 **ATOM** 573 CA ASP 231 53.730 38.339 14.531 1.00 19.93 **ATOM** 574 CB ASP 231 54.231 39.415 13.555 1.00 20.98 **ATOM** 575 CG ASP 231 53.754 40.817 13.915 1.00 24.11 **ATOM** 576 OD1 ASP 231 52.704 40.953 14.586 1.00 24.23 **ATOM** 577 OD2 ASP 231 54.443 41.784 13.522 1.00 25.90 **ATOM** 578 C **ASP** 231 54.097 36.962 13.982 1.00 19.27 **ATOM** 579 O **ASP** 231 53.266 36.279 13.380 1.00 17.80 **ATOM** 580 N PHE 232 55.357 36.582 14.163 1.00 18.91 **ATOM 581 CA PHE** 232 55.841 35.288 13.712 1.00 19.65 **ATOM** 582 CB PHE 232 57.308 35.078 14.104 1.00 18.14 **ATOM 583 CG PHE** 232 57.752 33.639 14.027 1.00 19.70 **ATOM** 584 CD1 PHE 232 57.895 33.005 12.799 1.00 19.18 **ATOM** 585 CD2 PHE 232 57.987 32.904 15.188 1.00 17.61 **ATOM** 232 58.259 31.660 12.723 1.00 19.86 586 CE1 PHE **ATOM** 587 CE2 PHE 232 58.350 31.560 15.126 1.00 18.98 **ATOM** 588 CZ PHE 232 58.487 30.935 13.892 1.00 19.46 **ATOM** 589 C PHE 232 54.996 34.179 14.320 1.00 21.02 **ATOM** 590 O PHE 232 54.458 33.339 13.598 1.00 20.88 **ATOM** 591 N ALA 233 54.863 34.202 15.645 1.00 21.64 **ATOM** 592 CA ALA 233 54.106 33.187 16.378 1.00 21.43 **ATOM** 593 CB ALA 233 54.223 33.443 17.868 1.00 18.72 **ATOM** 594 C ALA 233 52.643 33.134 15.955 1.00 23.15 **ATOM** 595 O **ALA** 233 52.043 32.062 15.857 1.00 21.76 **ATOM** 596 N LYS 234 52.083 34.307 15.689 1.00 25.54 **ATOM** 597 CA LYS 234 50.695 34.446 15.273 1.00 27.57 **ATOM** 598 CB LYS 234 50.360 35.935 15.146 1.00 30.65 **ATOM** 599 CG LYS 234 49.110 36.349 15.867 1.00 36.27 **ATOM** 234 600 CD LYS 49.192 35.988 17.334 1.00 41.19 601 CE LYS **ATOM** 234 47.800 35.677 17.890 1.00 43.69 **ATOM** 602 NZ LYS 234 47.119 34.565 17.147 1.00 44.98 **ATOM** 603 C LYS 234 50.443 33.739 13.933 1.00 27.70 **ATOM** 604 O LYS 234 49.355 33.200 13.693 1.00 28.42 **ATOM** 605 N LYS 235 51.458 33.732 13.074 1.00 26.06 **ATOM** 606 CA LYS 235 51.364 33.113 11.758 1.00 26.47 **ATOM** 607 CB LYS 235 52.350 33.791 10.819 1.00 25.23 **ATOM** 608 CG LYS 235 52.051 35.269 10.644 1.00 26.92 **ATOM** 609 CD LYS 235 53.017 35.959 9.697 1.00 28.41 **ATOM** 235 610 CE LYS 52.500 37.350 9.318 1.00 29.31 **ATOM** 611 NZ LYS 235 53.400 38.026 8.347 1.00 30.37 **ATOM** 612 C LYS 235 51.540 31.588 11.722 1.00 27.93 **ATOM** 613 O LYS 235 51.540 30.984 10.649 1.00 29.04 **ATOM** 614 N LEU 236 51.718 30.973 12.887 1.00 28.83 **ATOM** 615 CA LEU 236 51.866 29.524 12.986 1.00 29.05

ATOM 616 CB LEU 236 52.928 29.150 14.026 1.00 27.43 **ATOM** 617 CG LEU 236 54.352 29.660 13.774 1.00 25.84 **ATOM** 618 CD1 LEU 236 55.311 29.118 14.847 1.00 23.99 **ATOM** 619 CD2 LEU 236 54.801 29.236 12.389 1.00 23.86 **ATOM** 620 C LEU 236 50.513 28.948 13.392 1.00 31.19 **ATOM** 621 O. LEU 236 49.870 29.435 14.328 1.00 31.48 **ATOM** 622 N PRO 50.078 27.875 12.717 1.00 34.60 237 **ATOM** 623 CD PRO 237 50.829 27.156 11.668 1.00 35.04 ATOM 624 CA PRO 237 48.789 27.223 13.002 1.00 36.52 **ATOM** 625 CB PRO 237 48.751 26.081 11.981 1.00 37.48 **ATOM** 626 CG PRO 237 50.229 25.776 11.718 1.00 36.60 **ATOM** 627 C PRO 237 48.582 26.720 14.447 1.00 37.82 **ATOM** 628 O **PRO** 237 47.629 27.102 15.125 1.00 37.08 **ATOM** 629 N **MET** 238 49.495 25.893 14.935 1.00 40.42 **ATOM** 630 CA MET 238 49.366 25.350 16.285 1.00 43.00 631 CB MET **ATOM** 238 50.453 24.298 16.549 1.00 45.20 **ATOM** 632 CG MET 238 50.043 22.837 16.296 1.00 47.16 **ATOM 633 SD MET** 238 50.598 22.117 14.725 1.00 52.25 **ATOM** 634 CE MET 238 52.305 21.809 15.033 1.00 47.29 **ATOM** 635 C **MET** 238 49.389 26.389 17.414 1.00 43.25 **ATOM** 636 O **MET** 238 49.061 26.056 18.558 1.00 44.74 **ATOM** 637 N PHE 239 49.720 27.642 17.088 1.00 41.55 **ATOM** 638 CA PHE 239 49.825 28.716 18.091 1.00 37.31 **ATOM** 639 CB PHE 239 51.031 29.615 17.765 1.00 32.40 **ATOM** 640 CG PHE 239 51.293 30.673 18.795 1.00 27.12 **ATOM** 239 641 CD1 PHE 52.099 30.398 19.893 1.00 24.57 239 **ATOM** 642 CD2 PHE 50.705 31.933 18.686 1.00 24.70 **ATOM** 643 CE1 PHE 239 52.319 31.356 20.876 1.00 25.09 **ATOM** 644 CE2 PHE 239 50.915 32.901 19.659 1.00 25.90 **ATOM** 645 CZ PHE 239 51.726 32.612 20.761 1.00 24.52 **ATOM** PHE 48.574 29.582 18.352 1.00 36.84 646 C 239 **ATOM** 647 O PHE 239 48.136 29.728 19.497 1.00 34.67 **ATOM** 648 N SER 240 48.027 30.180 17.299 1.00 36.92 **ATOM** 649 CA SER 240 46.857 31.038 17.433 1.00 37.16 **ATOM** 650 CB SER 240 46.534 31.706 16:094 1.00 38.34 **ATOM** 651 C SER 240 45.627 30.304 17.981 1.00 37.30 **ATOM** 652 O SER 240 44.680 30.941 18.433 1.00 36.95 ATOM 653 N GLU 241 45.639 28.974 17.917 1.00 37.73 **ATOM** 654 CA GLU 241 44.531 28.155 18.418 1.00 38.44 **ATOM** 655 CB GLU 241 44.644 26.705 17.912 1.00 42.18 **ATOM** 656 CG GLU 241 44.290 26.471 16.436 1.00 48.01 **ATOM** 657 CD GLU 241 44.559 25.028 15.973 1.00 50.12 **ATOM** 658 OE1 GLU 241 44.375 24.088 16.779 1.00 51.14 659 OE2 GLU **ATOM** 241 44.957 24.838 14.799 1.00 50.68 **ATOM** 660 C 44.571 28.122 19.937 1.00 35.85 GLU 241 **ATOM** 661 O GLU 241 43.561 27.868 20.598 1.00 36.01 **ATOM** 662 N LEU 242 45.762 28.329 20.480 1.00 33.28

ATOM	663 CA LEU 242	45.959 28.296 21.920 1.00 31.31
ATOM		47.452 28.382 22.244 1.00 29.28
ATOM	665 CG LEU 242	, ====================================
ATOM	666 CD1 LEU 242	
ATOM	667 CD2 LEU 242	
ATOM	668 C LEU 242	45.223 29.390 22.676 1.00 30.10
ATOM	669 O LEU 242	44.874 30.434 22.116 1.00 28.69
ATOM	670 N PRO 243	44.867 29.115 23.937 1.00 30.09
ATOM	671 CD PRO 243	44.783 27.843 24.674 1.00 28.53
ATOM	672 CA PRO 243	44.183 30.200 24.640 1.00 31.01
ATOM	673 CB PRO 243	43.829 29.577 26.005 1.00 30.34
ATOM	674 CG PRO 243	44.640 28.300 26.093 1.00 29.25
ATOM	675 C PRO 243	45.195 31.356 24.774 1.00 31.71
ATOM	676 O PRO 243	46.412 31.128 24.840 1.00 30.69
ATOM	677 N CYS 244	44.694 32.585 24.804 1.00 32.36
ATOM	678 CA CYS 244	45.539 33.763 24.920 1.00 33.57
ATOM	679 CB CYS 244	44.675 35.028 25.050 1.00 37.62
ATOM	680 SG CYS 244	45.262 36.418 24.022 1.00 51.95
ATOM	681 C CYS 244	46.536 33.660 26.081 1.00 31.12
ATOM	682 O CYS 244	47.677 34.087 25.942 1.00 30.37
ATOM ATOM	683 N GLU 245 684 CA GLU 245	46.124 33.045 27.194 1.00 30.00
ATOM	684 CA GLU 245 685 CB GLU 245	46.993 32.877 28.366 1.00 29.62
ATOM	686 CG GLU 245	46.270 32.159 29.514 1.00 33.10 45.325 33.018 30.333 1.00 36.43
ATOM	687 CD GLU 245	
ATOM	688 OE1 GLU 245	43.882 32.940 29.860 1.00 37.87 42.989 33.006 30.730 1.00 37.36
ATOM	689 OE2 GLU 245	43.639 32.813 28.634 1.00 39.63
ATOM	690 C GLU 245	48.239 32.077 28.030 1.00 28.34
ATOM	691 O GLU 245	49.322 32.343 28.557 1.00 27.88
ATOM	692 N ASP 246	48.063 31.043 27.213 1.00 26.10
ATOM	693 CA ASP 246	49.182 30.212 26.798 1.00 25.23
ATOM	694 CB ASP 246	48.685 28.923 26.135 1.00 26.98
ATOM	695 CG ASP 246	48.146 27.912 27.137 1.00 29.13
ATOM	696 OD1 ASP 246	48.158 28.193 28.354 1.00 26.52
ATOM	697 OD2 ASP 246	47.712 26.824 25.696 1.00 31.38
ATOM	698 C ASP 246	50.065 30.983 25.826 1.00 23.57
ATOM	699 O ASP 246	51.288 30.993 25.955 1.00 22.61
ATOM	700 N GLN 247	49.431 31.630 24.852 1.00 23.23
ATOM	701 CA GLN 247	50.144 32.408 23.855 1.00 22.20
ATOM	702 CB GLN 247	49.159 33.178 22.991 1.00 22.06
ATOM	703 CG GLN 247	48.329 32.307 22.066 1.00 22.74
ATOM	704 CD GLN 247	47.435 33.141 21.169 1.00 24.91
ATOM	705 OE1 GLN 247	47.860 34.160 20.625 1.00 26.30
ATOM	706 NE2 GLN 247	46.186 32.732 21.035 1.00 25.65
ATOM	707 C GLN 247	51.098 33.374 24.528 1.00 22.10
ATOM	708 O GLN 247	52.280 33.454 24.182 1.00 23.07
ATOM	709 N ILE 248	50.587 34.076 25.527 1.00 23.27

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ATOM	710 CA ILE 248	51.379 35.042 26.276 1.00 23.21
ATOM	711 CB ILE 248	50.473 35.824 27.273 1.00 24.59
ATOM	712 CG2 ILE 248	51.304 36.682 28.242 1.00 24.09
ATOM	713 CG1 ILE 248	49.499 36.707 26.487 1.00 23.47
ATOM	714 CD1 ILE 248	48.413 37.323 27.341 1.00 23.84
ATOM	715 C ILE 248	52.568 34.387 26.986 1.00 22.27
ATOM	716 O ILE 248	53.705 34.833 26.829 1.00 22.06
ATOM	717 N ILE 249	52.321 33.313 27.729 1.00 21.40
ATOM	718 CA ILE 249	53.398 32.630 28.440 1.00 21.40
ATOM	719 CB ILE 249	52.850 31.438 29.279 1.00 23.53
ATOM	720 CG2 ILE 249	53.972 30.489 29.711 1.00 21.44
ATOM	721 CG1 ILE 249	52.098 31.963 30.500 1.00 22.76
ATOM	722 CD1 ILE 249	51.252 30.911 31.175 1.00 25.03
ATOM	723 C ILE 249	54.481 32.148 27.470 1.00 22.24
ATOM	724 O ILE 249	55.677 32.321 27.733 1.00 22.90
ATOM	725 N LEU 250	54.072 31.582 26.334 1.00 22.65
ATOM	726 CA LEU 250	55.028 31.079 25.345 1.00 21.40
ATOM	727 CB LEU 250	54.319 30.290 24.239 1.00 20.06
ATOM	728 CG LEU 250	53.566 29.038 24.677 1.00 20.22
ATOM	729 CD1 LEU 250	52.952 28.406 23.453 1.00 19.19
ATOM	730 CD2 LEU 250	54.494 28.050 25.386 1.00 18.52
ATOM	731 C LEU 250	55.850 32.209 24.736 1.00 20.82
ATOM	732 O LEU 250	57.069 32.094 24.603 1.00 20.27
ATOM	733 N LEU 251	55.179 33.302 24.384 1.00 22.14
ATOM	734 CA LEU 251	55.842 34.467 23.805 1.00 22.90
ATOM	735 CB LEU 251	54.806 35.543 23.471 1.00 22.76
ATOM	736 CG LEU 251	54.513 35.899 22.012 1.00 23.35
ATOM	737 CD1 LEU 251	55.347 35.103 21.047 1.00 22.38
ATOM	738 CD2 LEU 251	53.040 35.708 21.747 1.00 22.86
ATOM	739 C LEU 251	56.891 35.030 24.776 1.00 23.67
ATOM	740 O LEU 251	58.051 35.234 24.402 1.00 22.58
ATOM	741 N LYS 252	56.491 35.236 26.029 1.00 24.64
ATOM	742 CA LYS 252	57.395 35.754 27.057 1.00 26.22
ATOM	743 CB LYS 252	56.617 36.037 28.350 1.00 27.79
ATOM	744 CG LYS 252	55.351 36.838 28.093 1.00 32.69
ATOM	745 CD LYS 252	55.185 38.023 29.003 1.00 35.85
ATOM	746 CE LYS 252	54.773 37.626 30.397 1.00 39.34
ATOM	747 NZ LYS 252	54.477 38.870 31.168 1.00 44.60
ATOM	748 C LYS 252	58.566 34.793 27.312 1.00 25.26
ATOM	749 O LYS 252	59.701 35.222 27.555 1.00 26.67
ATOM ATOM	750 N GLY 253 751 CA GLY 253	58.306 33.497 27.195 1.00 23.97 50.356 32.521 27.404 1.00 23.00
ATOM		59.356 32.521 27.404 1.00 22.00
ATOM	752 C GLY 253 753 O GLY 253	60.397 32.429 26.292 1.00 23.10
ATOM	754 N CYS 254	61.568 32.165 26.585 1.00 25.12
ATOM	755 CA CYS 254	60.014 32.702 25.041 1.00 22.27
ATOM	756 CB CYS 254	60.944 32.584 23.908 1.00 20.91
YI OM	130 CD CIS 234	60.353 31.648 22.845 1.00 21.46
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757 SG CYS **ATOM** 254 58.992 32.385 21.893 1.00 22.92 **ATOM** 758 C **CYS** 254 61.354 33.869 23.201 1.00 19.77 **ATOM** 759 O **CYS** 254 62.215 33.834 22.316 1.00 19.88 **ATOM** 760 N **CYS** 255 60.731 34.984 23.561 1.00 19.56 **ATOM** 761 CA CYS 255 61.018 36.264 22.917 1.00 21.16 ATOM 762 CB CYS 255 60.292 37.407 23.634 1.00 21.21 **ATOM 763 SG CYS** 255 60.404 38.957 22.735 1.00 22.22 **ATOM** 764 C **CYS** 255 62.504 36.590 22.775 1.00 21.36 **ATOM** 765 O **CYS** 255 62.986 36.847 21.667 1.00 20.58 **ATOM** 766 N **MET** 256 63.232 36.574 23.887 1.00 20.52 **ATOM 767 CA MET** 256 64.657 36.874 23.835 1.00 20.07 **ATOM 768 CB MET** 256 65.255 36.967 25.253 1.00 20.39 **ATOM 769 CG MET** 256 66.744 37.360 25.267 1.00 19.20 **ATOM 770 SD MET** 256 67.066 38.952 24.447 1.00 20.26 **ATOM** 771 CE MET 256 68.856 38.971 24.375 1.00 18.47 **ATOM** *77*2 C **MET** 256 65.408 35.830 23.005 1.00 18.75 **ATOM** 773 O **MET** 256 66.305 36.164 22.225 1.00 18.15 **ATOM** 774 N **GLU** 257 65.035 34.568 23.170 1.00 19.00 **ATOM** 775 CA GLU 257 65.685 33.480 22.443 1.00 19.71 **ATOM** 776 CB GLU 257 65.104 32.145 22.882 1.00 21.15 **ATOM** 777 CG GLU 257 65.451 31.821 24.319 1.00 26.39 **ATOM** 257 778 CD GLU 64.513 30.820 24.929 1.00 30.75 **ATOM** 779 OE1 GLU 257 63.875 30.069 24.162 1.00 32.36 **ATOM** 780 OE2 GLU 257 64.415 30.783 26.172 1.00 33.70 **ATOM** 781 C GLU 257 65.545 33.648 20.940 1.00 18.54 **ATOM** 782 O GLU 66.521 33.506 20.197 1.00 17.58 257 **ATOM** 783 N ILE 258 64.336 33.977 20.497 1.00 17.78 **ATOM 784 CA ILE** 258 64.101 34.176 19.081 1.00 17.60 **ATOM** 785 CB ILE 258 62.590 34.267 18.765 1.00 16.35 **ATOM** 786 CG2 ILE 258 62.376 34.777 17.326 1.00 16.20 **ATOM** 787 CG1 ILE 258 61.935 32.884 18.980 1.00 17.24 **ATOM** 788 CD1 ILE 258 60.437 32.787 18.593 1.00 14.08 ILE 258 **ATOM** 789 C 64.872 35.408 18.595 1.00 19.11 **ATOM** 790 O ILE 258 65.609 35.326 17.601 1.00 19.02 **ATOM** 791 N **MET** 259 64.785 36.517 19.341 1.00 19.71 **ATOM 792 CA MET** 259 65.486 37.744 18.956 1.00 18.43 **ATOM 793 CB MET** 259 65.162 38.890 19.910 1.00 19.99 **ATOM 794 CG MET** 259 63.700 39.278 19.962 1.00 21.15 **ATOM 795 SD MET** 259 63.452 40.921 20.700 1.00 24.33 **ATOM 796 CE MET** 259 63.769 40.595 22.415 1.00 22.50 **ATOM** 797 C **MET** 259 66.993 37.540 18.888 1.00 18.64 **ATOM** 798 O **MET** 259 67.638 37.993 17.941 1.00 19.96 **ATOM** 799 N SER 260 67.556 36.858 19.884 1.00 17.37 **ATOM** 800 CA SER 260 68.993 36.592 19.915 1.00 16.76 **ATOM** 801 CB SER 260 69.387 35.840 21.195 1.00 17.25 **ATOM** 802 OG SER 69.078 36.589 22.346 1.00 22.89 260 **ATOM** 803 C SER 260 69.387 35.750 18.717 1.00 15.13

- ATOM	804 O SER 260	70.460 35.941 18.137 1.00 16.62
ATOM	805 N LEU 261	68.539 34.781 18.385 1.00 15.15
ATOM	806 CA LEU 261	68.802 33.900 17.262 1.00 15.31
ATOM	807 CB LEU 261	67.708 32.834 17.153 1.00 15.43
ATOM	808 CG LEU 261	67.652 32.014 15.858 1.00 15.82
ATOM	809 CD1 LEU 261	68.963 31.251 15.621 1.00 16.35
ATOM	810 CD2 LEU 261	66.470 31.060 15.937 1.00 13.72
ATOM	811 C LEU 261	68.839 34.741 16.001 1.00 16.31
ATOM	812 O LEU 261	69.766 34.619 15.194 1.00 16.68
ATOM	813 N ARG 262	67.848 35.620 15.853 1.00 16.47
ATOM	814 CA ARG 262	67.778 36.493 14.680 1.00 16.66
ATOM	815 CB ARG 262	66.475 37.279 14.693 1.00 16.00
ATOM	816 CG ARG 262	65.291 36.404 14.354 1.00 15.62
ATOM	817 CD ARG 262	63.995 37.167 14.378 1.00 17.31
ATOM	818 NE ARG 262	62.967 36.454 13.628 1.00 20.09
ATOM	819 CZ ARG 262	61.755 36.932 13.361 1.00 21.06
ATOM	820 NH1 ARG 262	61.390 38.136 13.787 1.00 19.02
ATOM	821 NH2 ARG 262	60.909 36.207 12.640 1.00 22.63
ATOM	822 C ARG 262	69.003 37.396 14.527 1.00 16.80
ATOM	823 O ARG 262	69.440 37.664 13.412 1.00 16.82
ATOM	824 N ALA 263	69.578 37.832 15.650 1.00 17.77
ATOM	825 CA ALA 263	70.795 38.647 15.637 1.00 18.41
ATOM	826 CB ALA 263	70.996 39.337 17.004 1.00 18.26
ATOM	827 C ALA 263	71.998 37.740 15.327 1.00 19.15
ATOM	828 O ALA 263	72.837 38.063 14.475 1.00 19.40
ATOM	829 N ALA 264	72.056 36.587 15.996 1.00 19.84
ATOM	830 CA ALA 264	73.155 35.633 15.818 1.00 20.35
ATOM	831 CB ALA 264	73.045 34.483 16.832 1.00 18.09
ATOM	832 C ALA 264	73.289 35.079 14.398 1.00 20.66
ATOM	833 O ALA 264	74.406 34.870 13.922 1.00 21.04
ATOM	834 N VAL 265	72.173 34.822 13.723 1.00 21.14
ATOM	835 CA VAL 265	72.249 34.299 12.358 1.00 22.96
ATOM	836 CB VAL 265	
ATOM	837 CG1 VAL 265	70.458 32.600 12.866 1.00 19.48
ATOM	838 CG2 VAL 265	69.838 34.708 11.698 1.00 18.96
ATOM	839 C VAL 265	72.718 35.387 11.382 1.00 24.66
ATOM	840 O VAL 265	73.026 35.103 10.224 1.00 26.03
ATOM	841 N ARG 266	72.777 36.628 11.858 1.00 25.11
ATOM	842 CA ARG 266	73.233 37.729 11.031 1.00 25.60
ATOM	843 CB ARG 266	72.187 38.819 10.964 1.00 24.09
ATOM	844 CG ARG 266	71.035 38.427 10.088 1.00 23.37
ATOM	845 CD ARG 266	69.998 39.492 10.098 1.00 24.80
ATOM	846 NE ARG 266	68.961 39.253 9.109 1.00 24.01
ATOM	847 CZ ARG 266	67.833 39.940 9.069 1.00 23.26
ATOM	848 NH1 ARG 266	67.613 40.880 9.970 1.00 24.16
ATOM	849 NH2 ARG 266	66.960 39.733 8.099 1.00 23.31
ATOM	850 C ARG 266	74.543 38.273 11.543 1.00 28.07

ATOM	851 O ARG 266	74.786 39.479 11.517 1.00 29.67
ATOM	852 N TYR 267	75.367 37.366 12.053 1.00 28.90
ATOM	853 CA TYR 267	
ATOM	854 CB TYR 267	77.223 36.584 13.434 1.00 29.98
ATOM	855 CG TYR 267	
ATOM		1.00 51.75
ATOM		80.544 37.705 14.950 1.00 31.29
ATOM		
ATOM		80.986 36.078 13.222 1.00 32.15
ATOM	860 CZ TYR 267	81.442 36.949 14.197 1.00 32.60
ATOM	861 OH TYR 267	82.801 37.052 14.389 1.00 34.13
ATOM	862 C TYR 267	77.570 37.900 11.343 1.00 31.17
ATOM	863 O TYR 267	77.543 37.086 10.426 1.00 30.91
ATOM	864 N ASP 268	78.361 38.966 11.336 1.00 33.09
ATOM	865 CA ASP 268	79.252 39.233 10.216 1.00 35.57
ATOM	866 CB ASP 268	79.085 40.679 9.747 1.00 39.39
ATOM	867 CG ASP 268	79.796 40.954 8.432 1.00 42.22
ATOM	868 OD1 ASP 268	79.426 40.331 7.412 1.00 46.07
ATOM	869 OD2 ASP 268	80.718 41.798 8.415 1.00 44.30
ATOM	870 C ASP 268	80.700 38.967 10.620 1.00 35.72
ATOM	871 O ASP 268	81.287 39.737 11.384 1.00 34.49
ATOM	872 N PRO 269	81.295 37.872 10.108 1.00 37.00
ATOM	873 CD PRO 269	80.712 36.887 9.182 1.00 36.77
ATOM	874 CA PRO 269	82.679 37.514 10.427 1.00 38.52
ATOM	875 CB PRO 269	82.905 36.239 9.611 1.00 37.06
ATOM	876 CG PRO 269	81.549 35.669 9.453 1.00 36.19
ATOM	877 C PRO 269	83.656 38.613 10.019 1.00 40.96
ATOM	878 O PRO 269	84.586 38.929 10.760 1.00 42.23
ATOM	879 N ALA 270	83.418 39.209 8.854 1.00 41.92
ATOM	880 CA ALA 270	84.277 40.272 8.342 1.00 42.08
ATOM	881 CB ALA 270	83.709 40.838 7.029 1.00 42.64
ATOM	882 C ALA 270	84.495 41.394 9.355 1.00 41.70
ATOM	883 O ALA 270	85.632 41.709 9.684 1.00 42.25
ATOM	884 N SER 271	83.408 41.970 9.865 1.00 41.87
ATOM	885 CA SER 271	83.495 43.073 10.830 1.00 40.75
ATOM	886 CB SER 271	82.454 44.143 10.500 1.00 40.60
ATOM	887 OG SER 271	81.150 43.590 10.464 1.00 40.31
ATOM	888 C SER 271	83.344 42.658 12.290 1.00 39.99
ATOM	889 O SER 271	83.484 43.487 13.194 1.00 38.77
ATOM	890 N ASP 272	83.042 41.381 12.508 1.00 38.94
ATOM	891 CA ASP 272	82.859 40.844 13.845 1.00 37.78
ATOM	892 CB ASP 272	84.182 40.904 14.625 1.00 38.86
ATOM	893 CG ASP 272	84.094 40.255 16.000 1.00 41.09
ATOM	894 OD1 ASP 272	83.342 39.275 16.173 1.00 41.64
ATOM	895 OD2 ASP 272	84.781 40.734 16.924 1.00 43.84
ATOM	896 C ASP 272	81.744 41.634 14.536 1.00 36.92
ATOM	897 O ASP 272	81.907 42.156 15.648 1.00 37.56

ATOM	898 N THR 273	80.603 41.723 13.865 1.00 33.65
ATOM	899 CA THR 273	79.469 42.443 14.425 1.00 31.57
ATOM	900 CB THR 273	79.246 43.790 13.695 1.00 31.69
ATOM	901 OG1 THR 273	79.087 43.557 12.289 1.00 30.71
ATOM	902 CG2 THR 273	80.426 44.730 13.922 1.00 31.53
ATOM	903 C THR 273	78.184 41.631 14.310 1.00 30.15
ATOM	904 O THR 273	78.104 40.697 13.504 1.00 30.10
ATOM	905 N LEU 274	77.213 41.942 15.164 1.00 27.09
ATOM	906 CA LEU 274	75.907 41.303 15.103 1.00 25.94
ATOM	907 CB LEU 274	75.396 40.936 16.496 1.00 24.47
ATOM	908 CG LEU 274	76.020 39.731 17.206 1.00 23.33
ATOM	909 CD1 LEU 274	75.436 39.631 18.602 1.00 21.14
ATOM	910 CD2 LEU 274	75.792 38.444 16.427 1.00 20.04
ATOM	911 C LEU 274	75.010 42.377 14.500 1.00 26.57
ATOM	912 O LEU 274	75.339 43.557 14.568 1.00 27.03
ATOM	913 N THR 275	73.914 41.987 13.865 1.00 26.60
ATOM	914 CA THR 275	73.009 42.966 13.285 1.00 26.48
ATOM	915 CB THR 275	72.786 42.717 11.781 1.00 26.52
ATOM	916 OG1 THR 275	74.044 42.719 11.097 1.00 28.67
ATOM	917 CG2 THR 275	71.919 43.799 11.198 1.00 27.35
ATOM	918 C THR 275	71.674 42.898 14.014 1.00 26.57
ATOM	919 O THR 275	71.069 41.825 14.121 1.00 28.50
ATOM	920 N LEU 276	71.236 44.026 14.564 1.00 25.18
ATOM	921 CA LEU 276	69.970 44.069 15.276 1.00 24.61
ATOM	922 CB LEU 276	70.057 44.987 16.506 1.00 23.61
ATOM	923 CG LEU 276	71.199 44.730 17.503 1.00 24.36
ATOM	924 CD1 LEU 276	71.039 45.654 18.709 1.00 19.91
ATOM	925 CD2 LEU 276	71.225 43.253 17.947 1.00 22.20
ATOM	926 C LEU 276	68.894 44.560 14.322 1.00 25.63
ATOM	927 O LEU 276	69.100 45.556 13.623 1.00 25.35
ATOM	928 N SER 277	67.787 43.814 14.249 1.00 25.94
ATOM	929 CA SER 277	66.634 44.141 13.403 1.00 24.61
ATOM	930 CB SER 277	65.874 45.335 13.987 1.00 21.96
ATOM	931 OG SER 277	65.368 45.029 15.273 1.00 19.68
ATOM	932 C SER 277	67.005 44.406 11.946 1.00 25.20
ATOM	933 O SER 277	66.350 45.199 11.267 1.00 25.21
ATOM	934 N GLY 278	68.067 43.747 11.489 1.00 27.08
ATOM	935 CA GLY 278	68.556 43.899 10.127 1.00 29.27
ATOM	936 C GLY 278	69.022 45.297 9.753 1.00 31.57
ATOM	937 O GLY 278	69.303 45.564 8.591 1.00 31.42
ATOM	938 N GLU 279	69.159 46.177 10.740 1.00 33.41
ATOM	939 CA GLU 279	69.558 47.560 10.484 1.00 34.84
ATOM	940 CB GLU 279	68.345 48.485 10.650 1.00 36.16
ATOM	941 CG GLU 279	67.843 48.606 12.090 1.00 38.08
ATOM	942 CD GLU 279	66.566 49.419 12.206 1.00 41.07
ATOM	943 OE1 GLU 279	66.475 50.279 13.108 1.00 41.98
ATOM	944 OE2 GLU 279	65.643 49.197 11.399 1.00 43.80

ATOM	945 C GLU 279	70.706 48.116 11.326 1.00 34.38
ATOM	946 O GLU 279	71.366 49.057 10.901 1.00 35.60
ATOM	947 N MET 280	70.944 47.565 12.511 1.00 33.43
ATOM	948 CA MET 280	72.014 48.085 13.358 1.00 32.27
ATOM	949 CB MET 280	71.443 48.544 14.702 1.00 31.81
ATOM	950 CG MET 280	72.471 49.181 15.637 1.00 29.76
ATOM	951 SD MET 280	71.813 49.482 17.289 1.00 29.63
ATOM	952 CE MET 280	70.592 50.735 16.989 1.00 24.91
ATOM	953 C MET 280	73.161 47.119 13.603 1.00 32.51
ATOM	954 O MET 280	72.995 46.117 14.303 1.00 32.78
ATOM	955 N ALA 281	74.321 47.408 13.021 1.00 31.74
ATOM	956 CA ALA 281	75.491 46.564 13.231 1.00 32.25
ATOM	957 CB ALA 281	76.494 46.740 12.108 1.00 30.91
ATOM	958 C ALA 281	76.091 47.006 14.563 1.00 33.09
ATOM	959 O ALA 281	76.261 48.202 14.805 1.00 34.06
ATOM	960 N VAL 282	76.358 46.053 15,447 1.00 33.78
ATOM	961 CA VAL 282	76.913 46.366 16.755 1.00 33.45
ATOM	962 CB VAL 282	75.858 46.208 17.885 1.00 34.92
ATOM	963 CG1 VAL 282	74.775 47.269 17.744 1.00 34.90
ATOM	964 CG2 VAL 282	75.246 44.806 17.860 1.00 34.39
ATOM	965 C VAL 282	78.119 45.514 17.087 1.00 33.93
ATOM	966 O VAL 282	78.202 44.347 16.702 1.00 35.11
ATOM	967 N LYS 283	79.071 46.123 17.777 1.00 33.49
ATOM	968 CA LYS 283	80.285 45.446 18.187 1.00 34.83
ATOM	969 CB LYS 283	81.446 46.445 18.183 1.00 35.96
ATOM	970 CG LYS 283	81.726 47.013 16.797 1.00 39.20
ATOM	971 CD LYS 283	82.621 48.245 16.844 1.00 43.38
ATOM	972 CE LYS 283	83.142 48.611 15.455 1.00 44.17
ATOM	973 NZ LYS 283	84.077 47.563 14.922 1.00 47.27
ATOM	974 C LYS 283	80.068 44.832 19.572 1.00 33.94
ATOM	975 O LYS 283	79.134 45.215 20.290 1.00 33.85
ATOM	976 N ARG 284	80.939 43.895 19.941 1.00 33.63
ATOM	977 CA ARG 284	80.873 43.184 21.217 1.00 34.00
ATOM	978 CB ARG 284	82.094 42.285 21.381 1.00 34.04
ATOM	979 CG ARG 284	82.332 41.369 20.219 1.00 36.31
ATOM	980 CD ARG 284	83.638 40.643 20.354 1.00 37.03
ATOM	981 NE ARG 284 982 CZ ARG 284	83.724 39.576 19.369 1.00 39.27
ATOM ATOM		83.323 38.326 19.583 1.00 40.07
ATOM	983 NH1 ARG 284 984 NH2 ARG 284	82.804 37.973 20.759 1.00 39.78
ATOM		83.434 37.428 18.613 1.00 40.16
ATOM	· · · · · ·	80.787 44.101 22.419 1.00 35.16
	986 O ARG 284	79.884 43.977 23.249 1.00 35.87
ATOM ATOM	987 N GLU 285	81.763 44.993 22.530 1.00 35.75
	988 CA GLU 285	81.827 45.939 23.632 1.00 36.86
ATOM ATOM	989 CB GLU 285	83.071 46.818 23.464 1.00 40.47
ATOM	990 CG GLU 285 991 CD GLU 285	83.202 47.973 24.444 1.00 49.23
VIOM	991 CD GLU 285	83.587 49.284 23.747 1.00 54.22

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ATOM	— 	84.784 49.657 23.760 1.00 55.37
ATOM		82.686 49.942 23.176 1.00 56.95
ATOM		80.552 46.785 23.684 1.00 34.45
ATOM		79.990 47.007 24.754 1.00 34.47
ATOM		80.046 47.166 22.515 1.00 32.27
ATOM		78.853 47.991 22.438 1.00 30.35
ATOM		78.615 48.472 21.006 1.00 33.34
ATOM		79.632 49.497 20.500 1.00 35.09
ATOM		79.293 50.023 19.108 1.00 38.42
ATOM		79.161 49.248 18.158 1.00 39.03
ATOM		79.156 51.339 18.982 1.00 37.82
ATOM	· · · · · · · · · · · · · · · · · · ·	77.605 47.308 22.970 1.00 29.57
ATOM		76.870 47.891 23.770 1.00 26.96
ATOM		77.352 46.080 22.524 1.00 29.50
ATOM		76.164 45.350 22.979 1.00 28.93
ATOM		75.831 44.182 22.029 1.00 27.14
ATOM		74.474 43.484 22.227 1.00 24.66
ATOM ATOM	· · · · · · · · · · · · · · · · · · ·	73.316 44.475 22.184 1.00 22.70
ATOM		74.297 42.413 21.163 1.00 25.17 76.303 44.874 24.433 1.00 28.10
ATOM		
ATOM	1012 O LLO 287	75.301 44.748 25.155 1.00 28.58 77.541 44.652 24.868 1.00 27.97
ATOM		77.808 44.218 26.230 1.00 27.57
ATOM	1015 CB LYS 288	79.270 43.800 26.376 1.00 28.93
ATOM	1016 CG LYS 288	79.603 43.254 27.750 1.00 32.46
ATOM	1017 CD LYS 288	81.015 42.725 27.826 1.00 33.48
ATOM	1018 CE LYS 288	81.205 41.878 29.071 1.00 35.76
ATOM	1019 NZ LYS 288	82.525 41.186 29.029 1.00 40.52
ATOM	1020 C LYS 288	77.497 45.341 27.220 1.00 29.15
ATOM	1021 O LYS 288	76.782 45.132 28.207 1.00 31.28
ATOM	1022 N ASN 289	77.996 46.539 26.933 1.00 28.58
ATOM	1023 CA ASN 289	77.794 47.692 27.811 1.00 28.40
ATOM	1024 CB ASN 289	78.815 48.775 27.485 1.00 28.28
ATOM	1025 CG ASN 289	80.224 48.329 27.770 1.00 31.30
ATOM	1026 OD1 ASN 289	80.445 47.442 28.601 1.00 33.02
ATOM ATOM	1027 ND2 ASN 289 1028 C ASN 289	81.190 48.928 27.087 1.00 30.49
ATOM	1028 C ASN 289 1029 O ASN 289	76.395 48.278 27.792 1.00 28.33
ATOM	1030 N GLY 290	76.005 48.977 28.724 1.00 28.36 75.638 47.977 26.740 1.00 26.71
ATOM	1031 CA GLY 290	74.286 48.487 26.606 1.00 23.27
ATOM	1032 C GLY 290	73.233 47.852 27.484 1.00 22.93
ATOM	1033 O GLY 290	72.063 48.219 27.399 1.00 23.84
ATOM	1034 N GLY 291	73.620 46.905 28.330 1.00 21.30
ATOM		72.637 46.290 29.199 1.00 20.38
ATOM	1036 C GLY 291	72.653 44.778 29.200 1.00 20.05
ATOM	1037 O GLY 291	72.190 44.165 30.147 1.00 21.91
ATOM	1038 N LEU 292	73.211 44.173 28.160 1.00 21.36

ATOM 1039 CA LEU 292 73.248 42.717 28.062 1.00 21.51 ATOM 1040 CB LEU 292 73.319 42.280 26.593 1.00 18.52 **ATOM** 1041 CG LEU 292 72.019 42.506 25.815 1.00 17.07 **ATOM** 1042 CD1 LEU 292 72.103 41.818 24.479 1.00 18.09 **ATOM** 1043 CD2 LEU 292 70.844 41.947 26.599 1.00 16.35 1044 C LEU 292 **ATOM** 74.347 42.046 28.872 1.00 22.17 **ATOM** 1045 O LEU 292 74.176 40.923 29.352 1.00 21.91 **ATOM** 1046 N GLY 293 75.479 42.724 29.011 1.00 23.76 ATOM 1047 CA GLY 293 76.588 42.169 29.760 1.00 23.92 **ATOM** 1048 C GLY 293 77.134 40.926 29.091 1.00 25.09 **ATOM** 1049 O **GLY** 293 77.362 40.919 27.883 1.00 26.51 **ATOM** 1050 N VAL 294 77.332 39.866 29.867 1.00 26.08 ATOM 1051 CA VAL 294 77.854 38.618 29.329 1.00 26.34 **ATOM** 1052 CB VAL 294 78.263 37.636 30.443 1.00 26.97 **ATOM** 1053 CG1 VAL 294 79.440 38.199 31.209 1.00 28.20 ATOM 1054 CG2 VAL 294 77.099 37.371 31.384 1.00 25.56 1055 C ATOM VAL 294 76.891 37.937 28.360 1.00 26.41 ATOM 1056 O VAL 294 77.315 37.097 27.568 1.00 27.65 **ATOM** 1057 N VAL 295 75.608 38.304 28.408 1.00 26.09 **ATOM** 1058 CA VAL 295 74.606 37.740 27.499 1.00 26.65 **ATOM** 1059 CB VAL 295 73.186 38.312 27.777 1.00 28.39 **ATOM** 1060 CG1 VAL 295 72.164 37.740 26.782 1.00 26.69 **ATOM** 1061 CG2 VAL 295 72.763 38.005 29.206 1.00 26.23 **ATOM** 1062 C VAL 295 75.035 38.089 26.069 1.00 25.83 **ATOM** 1063 O VAL 295 74.903 37.286 25.151 1.00 27.12 **ATOM** 1064 N SER 296 75.609 39.275 25.908 1.00 24.95 **ATOM** 1065 CA SER 296 76.097 39.725 24.619 1.00 26.17 **ATOM** 1066 CB SER 296 76.665 41.132 24.742 1.00 25.82 **ATOM** 296 1067 OG SER 77.253 41.554 23.525 1.00 26.64 **ATOM** 1068 C SER 296 77.196 38.783 24.142 1.00 28.63 **ATOM** 1069 O SER 296 77.241 38.420 22.963 1.00 29.19 **ATOM** 1070 N **ASP** 297 78.118 38.443 25.046 1.00 29.69 **ATOM** 1071 CA ASP 297 79.211 37.531 24.731 1.00 28.96 **ATOM** 1072 CB ASP 297 80.058 37.234 25.973 1.00 31.82 **ATOM** 1073 CG ASP 297 80.768 38.454 26.506 1.00 35.23 **ATOM** 1074 OD1 ASP 297 80.958 39.429 25.743 1.00 35.71 **ATOM** 1075 OD2 ASP 297 81.140 38.430 27.698 1.00 37.68 **ATOM** 1076 C ASP 297 78.605 36.227 24.247 1.00 27.63 **ATOM** 1077 O ASP 297 79.048 35.666 23.248 1.00 29.88 **ATOM** 1078 N ALA 298 77.581 35.762 24.952 1.00 25.15 ATOM 1079 CA ALA 298 76.909 34.527 24.592 1.00 24.49 **ATOM** 1080 CB ALA 298 75.811 34.224 25.594 1.00 21.91 **ATOM** 1081 C ALA 298 76.343 34.569 23.158 1.00 24.93 **ATOM** 1082 O **ALA 298** 76.589 33.654 22.357 1.00 24.83 **ATOM** 1083 N ILE 299 75.632 35.647 22.814 1.00 24.70 **ATOM** 1084 CA ILE 299 75.041 35.756 21.480 1.00 22.49 **ATOM** 1085 CB ILE 299 74.057 36.950 21.351 1.00 21.96

ATOM 1086 CG2 ILE 299 73.338 36.876 20.005 1.00 19.17 **ATOM** 1087 CG1 ILE 299 72.994 36.876 22.459 1.00 21.16 **ATOM** 1088 CD1 ILE 299 72.363 38.228 22.853 1.00 22.04 **ATOM** 1089 C ILE 299 76.127 35.829 20.428 1.00 22.33 **ATOM** 1090 O ILE 299 75.995 35.234 19.367 1.00 24.80 **ATOM** 1091 N PHE 300 77.209 36.538 20.724 1.00 21.92 **ATOM** 1092 CA PHE 300 78.322 36.641 19.785 1.00 23.08 **ATOM** 1093 CB PHE 300 79.385 37.636 20.278 1.00 24.08 **ATOM** 1094 CG PHE 300 79.249 39.017 19.686 1.00 24.18 **ATOM** 78.494 39.991 20.325 1.00 22.64 1095 CD1 PHE 300 **ATOM** 1096 CD2 PHE 79.857 39.331 18.471 1.00 23.76 300 **ATOM** 1097 CE1 PHE 300 78.347 41.253 19.770 1.00 22.38 **ATOM** 1098 CE2 PHE 300 79.715 40.596 17.904 1.00 23.21 1099 CZ PHE **ATOM** 300 78.957 41.558 18.554 1.00 22.46 1100 C 78.948 35.274 19.561 1.00 23.06 **ATOM** PHE 300 1101 O PHE **ATOM** 300 79.264 34.913 18.426 1.00 23.97 **ATOM** 1102 N GLU 301 79.113 34.506 20.636 1.00 23.75 **ATOM** 1103 CA GLU 301 79.694 33.169 20.525 1.00 24.16 **ATOM** 1104 CB GLU 301 79.884 32.545 21.902 1.00 23.03 1105 C GLU **ATOM** 301 78.776 32.302 19.672 1.00 23.62 **ATOM** 1106 O GLU 301 79.240 31.591 18.777 1.00 25.11 1107 N LEU 77.472 32.394 19.926 1.00 23.12 **ATOM** 302 **ATOM** 1108 CA LEU 302 76.495 31.624 19.166 1.00 23.56 **ATOM** 1109 CB LEU 302 75.082 31.865 19.701 1.00 21.75 **ATOM** 1110 CG LEU 302 73.953 31.120 18.979 1.00 22.61 **ATOM** 1111 CD1 LEU 302 74.084 29.612 19.193 1.00 22.31 1112 CD2 LEU 302 **ATOM** 72.611 31.604 19.485 1.00 19.27 1113 C LEU 302 ATOM 76.588 32.011 17.687 1.00 24.41 **ATOM** 302 1114 O LEU 76.670 31.140 16.814 1.00 24.63 **ATOM** 1115 N GLY 303 76.651 33.316 17.425 1.00 25.69 **ATOM** 1116 CA GLY 303 76.746 33.816 16.062 1.00 25.87 **ATOM** 1117 C GLY 303 77.975 33.288 15.338 1.00 28.63 **ATOM** 1118 O **GLY** 303 77.893 32.895 14.170 1.00 28.30 **ATOM** 1119 N LYS 304 79.116 33.279 16.023 1.00 29.53 **ATOM** 1120 CA LYS 304 80.360 32.791 15.437 1.00 31.18 **ATOM** 1121 CB LYS 304 81.529 32.931 16.418 1.00 34.79 **ATOM** 1122 CG LYS 304 82.157 34.307 16.506 1.00 40.28 **ATOM** 1123 CD LYS 304 83.441 34.262 17.332 1.00 44.37 1124 CE LYS **ATOM** 304 83.174 33.814 18.775 1.00 47.63 **ATOM** 1125 NZ LYS 304 82.459 34.847 19.592 1.00 48.83 **ATOM** 1126 C LYS 304 80.245 31.328 15.042 1.00 30.87 LYS **ATOM** 1127 O 304 80.632 30.944 13.932 1.00 29.53 **ATOM** 1128 N SER 305 79.720 30.518 15.961 1.00 30.46 1129 CA SER 305 **ATOM** 79.566 29.086 15.731 1.00 31.09 **ATOM** 1130 CB SER 305 79.243 28.370 17.041 1.00 29.83 **ATOM** 1131 OG SER 305 77.990 28.783 17.550 1.00 34.66 **ATOM** 1132 C SER 305 78.532 28.732 14.653 1.00 31.06

ATOM 1133 O 305 SER 78.745 27.799 13.872 1.00 31.84 **ATOM** 1134 N LEU 306 77.436 29.491 14.594 1.00 29.43 1135 CA LEU **ATOM** 306 76.378 29.258 13.611 1.00 28.39 **ATOM** 1136 CB LEU 306 75.121 30.055 13.962 1.00 26.05 **ATOM** 1137 CG LEU 306 74.306 29.573 15.157 1.00 26.33 **ATOM** 1138 CD1 LEU 306 73.061 30.430 15.285 1.00 26.22 **ATOM** 1139 CD2 LEU 306 73.924 28.110 14.985 1.00 25.86 **ATOM** 1140 C LEU 306 76.754 29.529 12.157 1.00 28.66 **ATOM** 1141 O LEU 306 76.116 29.001 11.253 1.00 28.58 **ATOM** SER 1142 N 307 77.786 30.338 11.931 1.00 29.72 **ATOM** 1143 CA SER 307 78.224 30.667 10.577 1.00 31.19 **ATOM** 1144 CB SER 307 79.466 31.556 10.617 1.00 30.15 ATOM 1145 OG SER 307 79.226 32.710 11.396 1.00 35.19 **ATOM** 1146 C **SER** 307 78.531 29.412 9.777 1.00 32.75 **ATOM** 1147 O SER 307 78.110 29.283 8.621 1.00 33.09 **ATOM** 1148 N ALA 308 79.248 28.482 10.407 1.00 33.36 **ATOM** 1149 CA ALA 308 79.626 27.223 9.769 1.00 34.50 **ATOM** 1150 CB ALA 308 80.636 26.473 10.637 1.00 33.55 **ATOM** 1151 C ALA 308 78.417 26.328 9.466 1.00 35.00 **ATOM ALA** 308 1152 O 78.469 25.501 8.550 1.00 37.10 ATOM 1153 N PHE 309 77.335 26.496 10.226 1.00 32.76 **ATOM** 1154 CA PHE 309 76.134 25.698 10.028 1.00 31.73 **ATOM** 1155 CB PHE 309 75.214 25.818 11.232 1.00 30.04 **ATOM** 1156 CG PHE 309 75.705 25.091 12.438 1.00 31.19 **ATOM** 1157 CD1 PHE 309 74.973 24.048 12.975 1.00 31.61 **ATOM** 1158 CD2 PHE 309 76.884 25.459 13.054 1.00 31.92 **ATOM** 1159 CE1 PHE 309 75.400 23.391 14.110 1.00 31.22 **ATOM** 1160 CE2 PHE 309 77.320 24.807 14.194 1.00 31.01 **ATOM** 1161 CZ PHE 309 76.577 23.771 14.720 1.00 30.47 ATOM 1162 C PHE 309 75.364 26.050 8.753 1.00 31.53 **ATOM** PHE 1163 O 309 74.516 25.269 8.310 1.00 31.28 ATOM 1164 N **ASN** 310 75.661 27.220 8.181 1.00 31.12 **ATOM** 1165 CA ASN 310 75.020 27.711 6.957 1.00 30.34 **ATOM** 1166 CB ASN 310 75.636 27.036 5.719 1.00 31.63 **ATOM** 1167 C **ASN** 310 73.511 27.492 7.003 1.00 29.40 **ATOM ASN** 1168 O 310 72.939 26.791 6.156 1.00 29.15 **ATOM** 1169 N LEU 311 72.875 28.055 8.026 1.00 27.60 71.435 27.907 **ATOM** 1170 CA LEU 311 8.205 1.00 28.23 **ATOM** 311 1171 CB LEU 71.021 28.313 9.621 1.00 27.41 **ATOM** 1172 CG LEU 311 71.603 27.558 10.822 1.00 26.80 **ATOM** 1173 CD1 LEU 311 70.949 28.078 12.112 1.00 25.05 **ATOM** 1174 CD2 LEU 311 71.360 26.062 10.662 1.00 24.72 **ATOM** 1175 C LEU 311 70.628 28.719 7.192 1.00 29.01 **ATOM** 1176 O LEU 311 71.040 29.808 6.782 1.00 30.66 ATOM 1177 N **ASP** 312 69.503 28.168 6.748 1.00 26.30 **ATOM** 1178 CA ASP 312 68.675 28.894 5.817 1.00 25.13 **ATOM** 1179 CB ASP 312 68.391 28.067 4.539 1.00 23.90

1180 CG ASP **ATOM** 67.438 26.890 4.754 1.00 21.34 312 **ATOM** 1181 OD1 ASP 312 66.959 26.631 5.868 1.00 22.47 ATOM 1182 OD2 ASP 312 67.154 26.206 3.758 1.00 22.18 1183 C ATOM **ASP** 312 67.419 29.379 6.542 1.00 24.49 **ATOM** 1184 O **ASP** 312 67.221 29.056 7.725 1.00 24.01 **ATOM** 1185 N° ASP 313 66.587 30.153 5.845 1.00 23.40 **ATOM** 1186 CA ASP 313 65.363 30.697 6.421 1.00 22.63 **ATOM** 1187 CB ASP 313 64.557 31.486 5.385 1.00 24.99 ATOM 1188 CG ASP 313 65.224 32.799 4.994 1.00 28.02 ATOM 1189 OD1 ASP 313 66.036 33.334 5.778 1.00 30.34 **ATOM** 1190 OD2 ASP 313 64.936 33.306 3.897 1.00 30.41 1191 C ATOM **ASP** 313 64.480 29.650 7.053 1.00 21.47 **ATOM** 1192 O **ASP** 313 63.853 29.917 8.082 1.00 21.76 **ATOM** 1193 N THR 314 64.407 28.474 6.435 1.00 19.16 ATOM 1194 CA THR 63.580 27.386 6.966 1.00 18.79 314 **ATOM** 1195 CB THR 314 63.398 26.240 5.913 1.00 19.68 **ATOM** 1196 OG1 THR 314 62.743 26.758 4.747 1.00 20.56 **ATOM** 1197 CG2 THR 314 62.558 25.112 6.482 1.00 18.84 **ATOM** 1198 C THR 64.133 26.818 8.293 1.00 15.38 314 **ATOM** 1199 O THR 314 63.383 26.538 9.223 1.00 14.08 **ATOM** 1200 N **GLU** 315 65.445 26.656 8.376 1.00 15.16 **ATOM** 1201 CA GLU 315 66.051 26.126 9.593 1.00 16.78 **ATOM** 1202 CB GLU 315 67.513 25.785 9.340 1.00 14.29 ATOM 1203 CG GLU 315 67.611 24.483 8.579 1.00 15.13 **ATOM** 1204 CD GLU 315 68.910 24.291 7.872 1.00 15.90 **ATOM** 1205 OE1 GLU 315 69.625 25.285 7.639 1.00 19.80 1206 OE2 GLU **ATOM** 315 69.211 23.129 7.527 1.00 19.34 **ATOM** 1207 C GLU 315 65.872 27.119 10.736 1.00 17.27 **ATOM** 1208 O **GLU** 315 65.457 26.742 11.836 1.00 17.46 1209 N VAL **ATOM** 316 66.081 28.399 10.440 1.00 17.12 **ATOM** 1210 CA VAL 316 65.897 29.441 11.446 1.00 16.92 **ATOM** 1211 CB VAL 316 66.336 30.828 10.918 1.00 15.89 **ATOM** 1212 CG1 VAL 316 66.062 31.921 11.962 1.00 14.60 **ATOM** 1213 CG2 VAL 316 67.811 30.785 10.579 1.00 15.95 **ATOM** 1214 C VAL 316 64.430 29.472 11.869 1.00 17.32 VAL ATOM 1215 O 316 64.131 29.582 13.055 1.00 18.11 **ATOM** 1216 N ALA 317 63.515 29.324 10.905 1.00 17.42 **ATOM** 1217 CA ALA 317 62.076 29.342 11.195 1.00 16.21 **ATOM** 1218 CB ALA 317 61.262 29.321 9.910 1.00 14.63 **ATOM** 1219 C ALA 317 61.656 28.181 12.079 1.00 16.84 317 **ATOM** 1220 O ALA 60.904 28.359 13.036 1.00 16.08 **ATOM** 1221 N LEU 318 62.146 26.990 11.759 1.00 17.27 **ATOM** 1222 CA LEU 318 61.783 25.804 12.526 1.00 17.88 **ATOM** 1223 CB LEU 318 62.141 24.525 11.748 1.00 17.58 **ATOM** 1224 CG LEU 318 61.331 24.333 10.439 1.00 16.87 61.837 23.155 9.658 1.00 15.79 **ATOM** 1225 CD1 LEU 318 **ATOM** 1226 CD2 LEU 318 59.860 24.149 10.728 1.00 14.08

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ATOM 1227 C LEU 318 62.394 25.852 13.932 1.00 18.20 **ATOM** 1228 O LEU 318 61.733 25.495 14.910 1.00 18.71 1229 N **ATOM** LEU 319 63.614 26.380 14.034 1.00 17.73 **ATOM** 1230 CA LEU 319 64.288 26.531 15.321 1.00 16.57 **ATOM** 1231 CB LEU 319 65.689 27.105 15.107 1.00 18.81 ATOM 1232 CG LEU 319 66.733 27.223 16.224 1.00 21.77 **ATOM** 1233 CD1 LEU 319 66.767 25.994 17.117 1.00 23.03 **ATOM** 1234 CD2 LEU 319 68.076 27.421 15.554 1.00 20.86 **ATOM** 1235 C LEU 319 63.433 27.471 16.160 1.00 16.07 **ATOM** 1236 O LEU 319 63.134 27.183 17.319 1.00 16.40 **ATOM** 1237 N GLN 320 62.948 28.546 15.545 1.00 13.91 ATOM 1238 CA GLN 320 62.101 29.490 16.253 1.00 13.86 **ATOM** 1239 CB GLN 320 61.782 30.697 15.373 1.00 13.26 **ATOM** 1240 CG GLN 320 62.994 31.553 15.080 1.00 12.17 ATOM 1241 CD GLN 320 62.691 32.802 14.253 1.00 13.98 **ATOM** 1242 OE1 GLN 320 63.597 33.568 13.950 1.00 15.61 **ATOM** 1243 NE2 GLN 320 61.436 32.993 13.862 1.00 13.85 **ATOM** 1244 C GLN 320 60.813 28.832 16.746 1.00 14.52 ATOM 1245 O GLN 320 60.367 29.087 17.864 1.00 15.12 **ATOM** 1246 N **ALA** 321 60.211 27.982 15.924 1.00 14.21 **ATOM** 1247 CA ALA 321 58.976 27.298 16.309 1.00 15.04 **ATOM** 1248 CB ALA 321 58.408 26.519 15.115 1.00 13.84 **ATOM** 1249 C ALA 321 59.217 26.349 17.487 1.00 15.98 **ATOM ALA** 1250 O 321 58.358 26.197 18.355 1.00 15.12 ATOM 1251 N VAL 322 60.373 25.687 17.488 1.00 16.63 ATOM 1252 CA VAL 322 60.720 24.757 18.557 1.00 18.74 **ATOM** 1253 CB VAL 322 62.012 23.943 18.231 1.00 19.42 ATOM 1254 CG1 VAL 322 62.493 23.154 19.455 1.00 19.45 **ATOM** 1255 CG2 VAL 322 61.745 22.986 17.083 1.00 19.05 **ATOM** 1256 C VAL 322 60.910 25.556 19.833 1.00 18.42 **ATOM** 1257 O VAL 322 60.421 25.164 20.886 1.00 19.46 **ATOM** 1258 N LEU 323 61.607 26.685 19.735 1.00 18.65 **ATOM** 1259 CA LEU 323 61.836 27.543 20.894 1.00 18.49 **ATOM** 1260 CB LEU 62.710 28.740 20.508 1.00 18.36 323 **ATOM** 323 1261 CG LEU 64.179 28.449 20.186 1.00 18.13 ATOM 1262 CD1 LEU 323 64.829 29.669 19.585 1.00 17.37 **ATOM** 1263 CD2 LEU 323 64.923 27.999 21.447 1.00 17.27 **ATOM** 1264 C LEU 323 60.499 28.029 21.454 1.00 18.38 **ATOM** LEU 1265 O 323 60.275 28.008 22.663 1.00 18.81 **ATOM** 1266 N LEU 324 59.595 28.406 20.557 1.00 18.67 **ATOM** 1267 CA LEU. 324 58.275 28.897 20.924 1.00 19.02 **ATOM** 1268 CB LEU 324 57.564 29.467 19.685 1.00 17.78 **ATOM** 1269 CG LEU 324 56.095 29.891 19.838 1.00 17.59 **ATOM** 1270 CD1 LEU 324 55.983 31.123 20.709 1.00 18.15 **ATOM** 1271 CD2 LEU 324 55.489 30.180 18.476 1.00 16.43 **ATOM** 1272 C 57.354 27.884 21.610 1.00 19.62 LEU 324 **ATOM** 1273 O LEU 324 56.735 28.185 22.633 1.00 19.40

ATOM 1274 N MET 325 57.224 26.701 21.029 1.00 21.14 **ATOM** 1275 CA MET 325 56.330 25.680 21.585 1.00 24.06 1276 CB MET **ATOM** 325 55.857 24.738 20.473 1.00 24.68 **ATOM** 1277 CG MET 325 55.169 25.444 19.303 1.00 24.49 1278 SD MET **ATOM** 325 53.759 26.457 19.820 1.00 26.18 **ATOM** 1279 CE MET 325 52.609 25.252 20.373 1.00 24.03 **ATOM** 1280 C **MET** 325 56.996 24.887 22.705 1.00 26.15 **ATOM** 1281 O **MET** 325 57.021 23.664 22.693 1.00 25.68 **ATOM** 1282 N SER 326 57.555 25.593 23.671 1.00 29.34 ATOM 1283 CA SER 326 58.232 24.938 24.774 1.00 32.40 ATOM 1284 CB SER 326 59.512 25.701 25.112 1.00 32.12 **ATOM** 1285 OG SER 326 60.127 25.173 26.272 1.00 36.86 **ATOM** 1286 C SER 326 57.317 24.831 25.996 1.00 34.04 **ATOM** 1287 O SER 326 56.532 25.741 26.280 1.00 33.24 1288 N **ATOM** THR 327 57.366 23.687 26.674 1.00 35.62 **ATOM** 1289 CA THR 327 56.560 23.486 27.867 1.00 36.88 **ATOM** 1290 CB THR 327 55.938 22.085 27.907 1.00 36.58 **ATOM** 1291 OG1 THR 327 56.953 21.094 27.714 1.00 38.58 1292 CG2 THR 327 ATOM 54.883 21.938 26.826 1.00 37.73 **ATOM** 1293 C THR 327 57.378 23.733 29.135 1.00 38.77 **ATOM** 1294 O THR 327 56.921 23.438 30.240 1.00 39.53 **ATOM** 1295 N **ASP** 328 58.593 24.260 28.972 1.00 41.25 **ATOM** 1296 CA ASP 328 59.473 24.573 30.099 1.00 43.20 **ATOM** 1297 CB ASP 328 60.940 24.698 29.655 1.00 46.47 1298 CG ASP ATOM 328 61.618 23.346 29.439 1.00 51.94 ATOM 1299 OD1 ASP 328 62.547 23.278 28.601 1.00 55.43 **ATOM** 1300 OD2 ASP 328 61.251 22.354 30.111 1.00 54.77 ATOM 1301 C **ASP** 328 59.001 25.905 30.653 1.00 43.79 **ATOM** 1302 O **ASP** 328 59.755 26.877 30.709 1.00 45.91 **ATOM** 1303 N ARG 329 57.724 25.967 30.995 1.00 43.55 **ATOM** 1304 CA ARG 329 57.143 27.178 31.542 1.00 43.04 ATOM 1305 CB ARG 329 56.398 27.997 30.482 1.00 43.87 ATOM 1306 CG ARG 329 57.258 28.740 29.504 1.00 40.87 ATOM 1307 CD ARG 329 57.545 27.886 28.314 1.00 39.52 **ATOM** 1308 NE ARG 329 58.301 28.643 27.341 1.00 38.90 **ATOM** 1309 CZ ARG 329 59.624 28.708 27.313 1.00 40.59 **ATOM** 1310 NH1 ARG 329 60.359 28.052 28.196 1.00 42.41 **ATOM** 1311 NH2 ARG 329 60.210 29.466 26.413 1.00 41.87 **ATOM** ARG 329 1312 C 56.152 26.817 32.609 1.00 43.00 **ATOM** 1313 O ARG 329 55.600 25.716 32.628 1.00 43.66 **ATOM** 330 1314 N SER 55.886 27.797 33.456 1.00 41.58 **ATOM** 1315 CA SER 330 54.953 27.641 34.538 1.00 40.11 **ATOM** 55.491 28.362 35.777 1.00 40.38 1316 CB SER 330 **ATOM** 1317 C SER 330 53.602 28.223 34.103 1.00 38.99 ATOM 1318 O SER 330 53.553 29.172 33.320 1.00 39.22 52.517 27.581 34.529 1.00 37.52 **ATOM** 1319 N GLY 331 **ATOM** 1320 CA GLY 331 51.176 28.063 34.232 1.00 35.64

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ATOM 1321 C GLY 331 50.493 27.782 32.906 1.00 35.14 **ATOM** 1322 O **GLY** 331 49.439 28.363 32.640 1.00 34.48 1323 N LEU **ATOM** 332 51.059 26.925 32.066 1.00 34.54 1324 CA LEU **ATOM** 332 50.424 26.637 30.780 1.00 34.59 **ATOM** 1325 CB LEU 332 51.394 25.942 29.828 1.00 33.09 **ATOM** 1326 CG LEU 332 52.532 26.765 29.236 1.00 32.72 **ATOM** 1327 CD1 LEU 332 53.473 25.834 28.497 1.00 30.29 **ATOM** 1328 CD2 LEU 332 51.987 27.844 28.313 1.00 29.20 ATOM 1329 C LEU 332 49.191 25.763 30.969 1.00 35.14 ATOM 1330 O LEU 332 49.178 24.874 31.811 1.00 35.96 **ATOM** 1331 N LEU 333 48.153 26.076 30.204 1.00 35.65 1332 CA LEU ATOM 333 46.898 25.345 30.215 1.00 37.97 **ATOM** 1333 CB LEU 333 45.743 26.271 29.796 1.00 40.71 **ATOM** 1334 CG LEU 333 45.389 27.483 30.670 1.00 43.46 **ATOM** 1335 CD1 LEU 333 44.713 28.620 29.882 1.00 42.72 **ATOM** 1336 CD2 LEU 333 44.487 27.021 31.806 1.00 45.25 **ATOM** 1337 C LEU 333 46.952 24.115 29.300 1.00 37.78 **ATOM** 1338 O LEU 333 46.695 22.991 29.720 1.00 37.65 47.361 24.323 28.060 1.00 38.65 **ATOM** 1339 N CYA 334 ATOM 1340 CA CYA 334 47.413 23.249 27.073 1.00 40.91 **ATOM** 1341 CB CYA 46.936 23.788 25.721 1.00 47.35 334 **ATOM** 1342 SG CYA 334 45.406 24.693 25.867 1.00 52.24 **ATOM** 1343 AS CYA 334 44.066 22.890 25.562 1.00 70.72 **ATOM** 1344 C CYA 334 48.778 22.588 26.901 1.00 39.85 **ATOM** 1345 O **CYA** 334 49.287 22.473 25.775 1.00 39.54 **ATOM** 1346 N VAL 335 49.329 22.078 27.997 1.00 37.67 1347 CA VAL 335 ATOM 50.641 21.432 27.967 1.00 36.07 **ATOM** 1348 CB VAL 335 51.019 20.905 29.384 1.00 33.70 **ATOM** 1349 CG1 VAL 335 52.434 20.332 29.401 1.00 33.70 **ATOM** 1350 CG2 VAL 335 50.913 22.028 30.387 1.00 31.84 ATOM 1351 C VAL 335 50.734 20.334 26.885 1.00 36.09 **ATOM** 1352 O VAL 335 51.662 20.335 26.064 1.00 34.41 **ATOM** 1353 N ASP 336 49.747 19.444 26.833 1.00 35.95 **ATOM** 1354 CA ASP 336 49.748 18.372 25.844 1.00 36.34 **ATOM** 1355 CB ASP 336 48.591 17.394 26.091 1.00 41.36 1356 CG ASP 336 **ATOM** 48.613 16.206 25.129 1.00 46.23 ATOM 1357 OD1 ASP 336 47.615 16.021 24.392 1.00 49.55 **ATOM** 1358 OD2 ASP 336 49.639 15.470 25.097 1.00 48.07 **ATOM** 1359 C ASP 336 49.727 18.846 24.390 1.00 33.05 **ATOM** 1360 O ASP 336 50.527 18.377 23.573 1.00 32.33 **ATOM** 1361 N LYS 337 48.794 19.743 24.076 1.00 29.57 **ATOM** 1362 CA LYS 337 48.661 20.286 22.723 1.00 27.76 **ATOM** 1363 CB LYS 337 47.520 21.313 22.689 1.00 27.09 **ATOM** 1364 C LYS 337 49.988 20.941 22.286 1.00 27.64 LYS 337 **ATOM** 1365 O 50.472 20.713 21.173 1.00 26.09 50.597 21.688 23.208 1.00 25.90 **ATOM** 1366 N ILE 338 **ATOM** 1367 CA ILE 338 51.852 22.394 22.971 1.00 24.21

ATOM	1368 CB ILE 338	52.128 23.391 24.122 1.00 23.30
ATOM	1369 CG2 ILE 338	53.500 24.048 23.958 1.00 21.75
ATOM	1370 CG1 ILE 338	51.014 24.448 24.155 1.00 21.19
ATOM	1371 CD1 ILE 338	51.055 25.393 25.361 1.00 21.39
ATOM	1372 C ILE 338	53.041 21.451 22.782 1.00 25.55
ATOM	1373 O' ILE 338	53.861 21.640 21.875 1.00 24.74
ATOM	1374 N GLU 339	53.124 20.421 23.622 1.00 27.43
ATOM	1375 CA GLU 339	54.220 19.448 23.536 1.00 27.60
ATOM	1376 CB GLU 339	54.201 18.512 24.755 1.00 27.21
ATOM	1377 C GLU 339	54.112 18.650 22.236 1.00 26.85
ATOM	1378 O GLU 339	55.119 18.385 21.581 1.00 26.71
ATOM	1379 N LYS 340	52.888 18.276 21.872 1.00 27.04
ATOM	1380 CA LYS 340	52.663 17.515 20.654 1.00 28.19
ATOM	1381 CB LYS 340	51.210 17.008 20.609 1.00 28.67
ATOM	1382 C LYS 340	53.002 18.402 19.439 1.00 27.96
ATOM	1383 O LYS 340	53.558 17.934 18.436 1.00 27.48
ATOM	1384 N SER 341	52.746 19.700 19.567 1.00 28.32
ATOM	1385 CA SER 341	53.058 20.662 18.514 1.00 28.02
ATOM ATOM	1386 CB SER 341 1387 OG SER 341	52.457 22.022 18.867 1.00 31.25
ATOM	1387 OG SER 341 1388 C SER 341	52.880 23.029 17.965 1.00 37.69 54.578 20.773 18.350 1.00 26.01
ATOM	1389 O SER 341	54.578 20.773 18.350 1.00 26.01 55.096 20.717 17.234 1.00 25.06
ATOM	1390 N GLN 342	55.297 20.899 19.462 1.00 25.71
ATOM	1391 CA GLN 342	56.750 20.993 19.398 1.00 25.71
ATOM	1392 CB GLN 342	57.356 21.254 20.777 1.00 24.17
ATOM	1393 CG GLN 342	58.834 21.590 20.703 1.00 25.09
ATOM	1394 CD GLN 342	59.476 21.677 22.057 1.00 26.93
ATOM	1395 OE1 GLN 342	59.479 20.704 22.810 1.00 27.77
ATOM	1396 NE2 GLN 342	60.022 22.839 22.386 1.00 24.61
ATOM	1397 C GLN 342	57.354 19.715 18.806 1.00 25.69
ATOM	1398 O GLN 342	58.356 19.771 18.075 1.00 24.99
ATOM	1399 N GLU 343	56.753 18.569 19.127 1.00 25.00
ATOM		57.222 17.280 18.610 1.00 25.34
ATOM	1401 CB GLU 343	56.411 16.118 19.245 1.00 25.90
ATOM	1402 C GLU 343	57.089 17.276 17.076 1.00 24.32
ATOM	1403 O GLU 343	58.021 16.891 16.365 1.00 23.99
ATOM	1404 N ALA 344	55.961 17.789 16.587 1.00 23.56
ATOM	1405 CA ALA 344	55.701 17.875 15.153 1.00 22.85
ATOM	1406 CB ALA 344	54.320 18.451 14.917 1.00 22.64
ATOM	1407 C ALA 344	56.768 18.743 14.489 1.00 22.77
ATOM	1408 O ALA 344	57.355 18.360 13.477 1.00 22.08
ATOM	1409 N TYR 345	57.057 19.893 15.092 1.00 21.89
ATOM	1410 CA TYR 345	58.075 20.792 14.550 1.00 21.18
ATOM	1411 CB TYR 345	58.108 22.119 15.313 1.00 20.27
ATOM ATOM	1412 CG TYR 345	57.048 23.078 14.856 1.00 17.45
ATOM ATOM	1413 CD1 TYR 345 1414 CE1 TYR 345	56.001 23.431 15.698 1.00 17.99 54.992 24.253 15.270 1.00 10.97
WI OIAI	TITE CELLIK 343	54.992 24.253 15.270 1.00 19.97

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ATOM	1415 CD2 TYR 345	57.063 23.589 13.562 1.00 19.11
ATOM	1416 CE2 TYR 345	56.055 24.424 13.116 1.00 19.14
ATOM	1417 CZ TYR 345	55.017 24.749 13.972 1.00 20.78
ATOM		53.983 25.539 13.530 1.00 20.70
ATOM	_ · · -	59.454 20.167 14.583 1.00 20.96
ATOM	1420 O TYR 345	60.221 20.314 13.632 1.00 22.29
ATOM	1421 N LEU 346	59.778 19.480 15.677 1.00 20.82
ATOM	1422 CA LEU 346	61.079 18.838 15.817 1.00 20.18
ATOM	1423 CB LEU 346	61.216 18.203 17.205 1.00 21.04
ATOM	•	61.606 19.158 18.335 1.00 21.25
ATOM	1425 CD1 LEU 346	61.226 18.595 19.685 1.00 20.95
ATOM	1426 CD2 LEU 346	63.099 19.438 18.267 1.00 19.90
ATOM	1427 C LEU 346	61.317 17.806 14.716 1.00 20.19
ATOM	1428 O LEU 346	62.407 17.755 14.142 1.00 20.69
ATOM	1429 N LEU 347	60.290 17.016 14.390 1.00 22.00
ATOM ATOM	1430 CA LEU 347 1431 CB LEU 347	60.406 15.994 13.344 1.00 21.81 59.199 15.051 13.366 1.00 24.03
ATOM	1431 CB LEU 347	59.199 15.051 13.366 1.00 24.03 59.301 13.805 14.250 1.00 26.28
ATOM	1432 CO LEO 347	57.964 13.072 14.277 1.00 27.79
ATOM	1434 CD2 LEU 347	60.409 12.889 13.728 1.00 24.78
ATOM	1435 C LEU 347	60.544 16.623 11.966 1.00 20.50
ATOM	1436 O LEU 347	61.351 16.179 11.143 1.00 21.39
ATOM	1437 N ALA 348	59.767 17.674 11.727 1.00 20.84
ATOM	1438 CA ALA 348	59.788 18.381 10.456 1.00 18.12
ATOM	1439 CB ALA 348	58.729 19.480 10.457 1.00 18.49
ATOM	1440 C ALA 348	61.168 18.963 10.269 1.00 17.53
ATOM	1441 O ALA 348	61.785 18.781 9.228 1.00 18.78
ATOM	1442 N PHE 349	61.677 19.569 11.338 1.00 19.55
ATOM	1443 CA PHE 349	63.001 20.196 11.389 1.00 19.84
ATOM	1444 CB PHE 349	63.188 20.823 12.786 1.00 18.68
ATOM	1445 CG PHE 349	64.380 21.758 12.917 1.00 19.12
ATOM	1446 CD1 PHE 349	65.234 22.008 11.851 1.00 19.95
ATOM ATOM	1447 CD2 PHE 349 1448 CE1 PHE 349	64.618 22.420 14.126 1.00 20.06 66.294 22.905 11.971 1.00 18.99
ATOM	1448 CE1 PHE 349	65.674 23.317 14.261 1.00 16.79
ATOM	1450 CZ PHE 349	66.516 23.562 13.184 1.00 18.91
ATOM	1451 C PHE 349	64.108 19.170 11.103 1.00 20.44
ATOM	1452 O PHE 349	64.980 19.401 10.260 1.00 19.83
ATOM	1453 N GLU 350	64.064 18.032 11.794 1.00 23.59
ATOM	1454 CA GLU 350	65.077 16.995 11.610 1.00 23.46
ATOM	1455 CB GLU 350	64.830 15.845 12.584 1.00 25.26
ATOM	1456 CG GLU 350	65.694 14.644 12.288 1.00 31.98
ATOM	1457 CD GLU 350	65.526 13.482 13.257 1.00 35.49
ATOM	1458 OE1 GLU 350	66.560 12.853 13.555 1.00 40.26
ATOM	1459 OE2 GLU 350	64.380 13.173 13.689 1.00 36.23
ATOM	1460 C GLU 350	65.083 16.489 10.165 1.00 21.12
ATOM	1461 O GLU 350	66.133 16.384 9.526 1.00 19.81

ATOM	1462 N HIS 351	63.888 16.234 9.651 1.00 21.98
ATOM	1463 CA HIS 351	63.694 15.751 8.292 1.00 21.31
ATOM	1464 CB HIS 351	62.238 15.321 8.107 1.00 21.76
ATOM	1465 CG HIS 351	61.839 14.160 8.967 1.00 22.08
ATOM	1466 CD2 HIS 351	62.578 13.317 9.728 1.00 22.65
ATOM	1467 ND1 HIS 351	60.532 13.751 9.115 1.00 22.37
ATOM	1468 CE1 HIS 351	60.478 12.716 9.930 1.00 21.44
ATOM	1469 NE2 HIS 351	61.705 12.429 10.314 1.00 20.85
ATOM	1470 C HIS 351	64.117 16.815 7.275 1.00 21.18
ATOM	1471 O HIS 351	64.683 16.489 6.231 1.00 22.65
ATOM	1472 N TYR 352	63.915 18.088 7.602 1.00 19.79
ATOM	1473 CA TYR 352	64.327 19.146 6.697 1.00 18.72
ATOM	1474 CB TYR 352	63.768 20.502 7.122 1.00 19.55
ATOM	1475 CG TYR 352	64.140 21.580 6.137 1.00 19.27
ATOM	1476 CD1 TYR 352	63.556 21.623 4.867 1.00 19.29
ATOM	1477 CE1 TYR 352	63.961 22.555 3.927 1.00 17.55
ATOM	1478 CD2 TYR 352	65.132 22.507 6.438 1.00 18.91
ATOM	1479 CE2 TYR 352	65.545 23.443 5.503 1.00 17.30
ATOM	1480 CZ TYR 352	64.954 23.459 4.256 1.00 18.41
ATOM	1481 OH TYR 352	65.355 24.384 3.334 1.00 19.40
ATOM	1482 C TYR 352	65.849 19.182 6.687 1.00 19.31
ATOM	1483 O TYR 352	66.479 19.333 5.639 1.00 20.25
ATOM	1484 N VAL 353	66.446 19.017 7.858 1.00 21.25
ATOM	1485 CA VAL 353	67.899 18.993 7.960 1.00 22.03
ATOM	1486 CB VAL 353	68.348 18.880 9.450 1.00 22.60
ATOM	1487 CG1 VAL 353	69.843 18.635 9.550 1.00 20.34
ATOM	1488 CG2 VAL 353	67.997 20.167 10.183 1.00 22.61
ATOM	1489 C VAL 353	68.442 17.827 7.108 1.00 22.74
ATOM	1490 O VAL 353	69.448 17.985 6.398 1.00 23.44
ATOM	1491 N ASN 354	67.773 16.674 7.165 1.00 22.30
ATOM	1492 CA ASN 354	68.185 15.508 6.373 1.00 23.56
ATOM	1493 CB ASN 354	67.241 14.320 6.603 1.00 22.26
ATOM	1494 CG ASN 354	67.374 13.715 7.981 1.00 23.06
ATOM	1495 OD1 ASN 354	68.406 13.843 8.628 1.00 25.79
ATOM	1496 ND2 ASN 354	66.327 13.044 8.435 1.00 21.07
ATOM	1497 C ASN 354	68.134 15.877 4.888 1.00 25.10
ATOM	1498 O ASN 354	69.024 15.534 4.111 1.00 26.70
ATOM	1499 N HIS 355	67.067 16.568 4.503 1.00 24.50
ATOM	1500 CA HIS 355	66.881 16.986 3.123 1.00 24.46
ATOM	1501 CB HIS 355	65.557 17.750 2.969 1.00 26.07
ATOM	1502 CG HIS 355	65.365 18.337 1.604 1.00 28.28
ATOM	1503 CD2 HIS 355	65.918 19.422 1.018 1.00 28.10
ATOM	1504 ND1 HIS 355	64.600 17.724 0.632 1.00 26.32
ATOM	1505 CE1 HIS .355	64.706 18.407 -0.499 1.00 27.71
ATOM	1506 NE2 HIS 355	65.502 19.435 -0.288 1.00 27.79
ATOM	1507 C HIS 355	68.022 17.857 2.624 1.00 24.07
ATOM	1508 O HIS 355	68.460 17.729 1.484 1.00 23.54

ATOM 1509 N ARG 356 68.463 18.774 3.471 1.00 25.31 **ATOM** 1510 CA ARG 356 69.523 19.714 3.130 1.00 25.69 ATOM 1511 CB ARG 69.561 20.820 356 4.168 1.00 24.06 **ATOM** 1512 CG ARG 356 68.337 21.682 4.094 1.00 23.23 **ATOM** 1513 CD ARG 356 68.670 22.973 3.424 1.00 25.91 ATOM 1514 NE ARG 356 69.447 23.814 4.322 1.00 24.87 ATOM 1515 CZ ARG 356 70.325 24.726 3.928 1.00 25.05 ATOM 1516 NH1 ARG 356 70.546 24.920 2.640 1.00 24.97 ATOM 1517 NH2 ARG 356 70.978 25.453 4.831 1.00 25.62 ATOM 1518 C ARG 356 70.900 19.109 2.949 1.00 27.73 ATOM 1519 O ARG 356 71.724 19.645 2.208 1.00 28.38 **ATOM** 1520 N LYS 357 71.179 18.048 3.693 1.00 29.45 **ATOM** 1521 CA LYS 357 72.457 17.355 3.588 1.00 31.35 **ATOM** 1522 CB LYS 357 72.503 16.566 2.270 1.00 32.80 ATOM 1523 CG LYS 357 71.290 15.650 2.103 1.00 35.78 **ATOM** 1524 CD LYS 357 71.264 14.927 0.778 1.00 39.43 ATOM 1525 CE LYS 357 70.121 13.918 0.739 1.00 42.93 1526 NZ LYS **ATOM** 357 70.162 13.074 -0.498 1.00 45.97 **ATOM** 1527 C LYS 357 73.692 18.247 3.743 1.00 31.34 ATOM 1528 O LYS 357 74.489 18.390 2.818 1.00 32.65 **ATOM** 1529 N HIS 358 73.837 18.861 4.913 1.00 30.72 **ATOM** 1530 CA HIS 358 74.995 19.706 5.186 1.00 31.49 **ATOM** 1531 CB HIS 358 74.895 20.322 6.579 1.00 29.13 73.882 21.415 **ATOM** 1532 CG HIS 358 6.688 1.00 25.30 **ATOM** 1533 CD2 HIS 358 74.026 22.760 6.646 1.00 24.90 **ATOM** 1534 ND1 HIS 358 72.543 21.175 6.892 1.00 24.54 **ATOM** 1535 CE1 HIS 358 71.901 22.324 6.975 1.00 23.68 **ATOM** 1536 NE2 HIS 358 72.777 23.302 6.830 1.00 25.28 **ATOM** 1537 C HIS 358 76.235 18.831 5.161 1.00 33.38 **ATOM** 1538 O HIS 358 76.166 17.647 5.495 1.00 35.46 ATOM 1539 N ASN 359 77.366 19.399 4.768 1.00 35.34 **ATOM** 1540 CA ASN 359 78.606 18.636 4.746 1.00 38.17 **ATOM** 1541 CB ASN 359 79.544 19.150 3.646 1.00 37.84 **ATOM** 1542 C ASN 359 79.236 18.825 6.120 1.00 39.85 80.317 19.406 6.240 1.00 42.72 **ATOM** 1543 O ASN 359 **ATOM** 1544 N ILE 360 78.510 18.411 7.159 1.00 39.01 ATOM 1545 CA ILE 360 78.968 18.526 8.549 1.00 36.72 **ATOM** 1546 CB ILE 360 78.351 19.752 9.264 1.00 37.69 **ATOM** 1547 CG2 ILE 360 78.802 19.793 10.722 1.00 37.56 ATOM 1548 CG1 ILE 360 78.735 21.049 8.549 1.00 37.68 **ATOM** 1549 CD1 ILE 360 77.970 22.253 9.041 1.00 38.40 **ATOM** 1550 C ILE 360 78.524 17.278 9.303 1.00 35.15 77.343 16.931 9.314 1.00 33.75 **ATOM** 1551 O ILE 360 **ATOM** 1552 N PRO 361 79.475 16.564 9.912 1.00 34.64 **ATOM** 1553 CD PRO 361 80.930 16.785 9.873 1.00 35.59 **ATOM** 79.138 15.349 10.660 1.00 33.92 1554 CA PRO 361 **ATOM** 80.513 14.768 11.014 1.00 35.27 1555 CB PRO 361

ATOM 1556 CG PRO 361 81.412 15.972 11.048 1.00 35.97 **ATOM** 1557 C PRO 361 78.292 15.618 11.909 1.00 30.95 **ATOM** 1558 O **PRO** 361 78.555 16.554 12.653 1.00 31.50 **ATOM** 1559 N HIS 362 77.269 14.793 12.112 1.00 28.75 **ATOM** 1560 CA HIS 362 76.378 14.900 13.263 1.00 30.25 **ATOM** 1561 CB HIS 362 77.152 14.612 14.548 1.00 31.20 ATOM 1562 CG HIS 362 78.075 13.441 14.440 1.00 33.72 **ATOM** 1563 CD2 HIS 362 77.826 12.122 14.275 1.00 34.55 **ATOM** 1564 ND1 HIS 362 79.449 13.569 14.469 1.00 35.55 **ATOM** 1565 CE1 HIS 362 80.006 12.377 14.322 1.00 35.28 **ATOM** 1566 NE2 HIS 362 79.040 11.484 14.204 1.00 37.61 **ATOM** 1567 C HIS 362 75.742 16.275 13.368 1.00 29.44 HIS **ATOM** 1568 O 362 75.521 16.769 14.472 1.00 29.93 **ATOM** 1569 N PHE 363 75.397 16.856 12.222 1.00 29.22 ATOM 1570 CA PHE 363 74.803 18.188 12.160 1.00 27.72 1571 CB PHE **ATOM** 363 74.446 18.538 10.709 1.00 26.85 **ATOM** 1572 CG PHE 363 73.901 19.931 10.532 1.00 27.48 **ATOM** 1573 CD1 PHE 363 74.758 21.017 10.391 1.00 27.76 ATOM 1574 CD2 PHE 363 72.523 20.157 10.513 1.00 27.45 **ATOM** 1575 CE1 PHE 363 74.244 22.313 10.234 1.00 28.56 1576 CE2 PHE 363 **ATOM** 72.001 21.446 10.357 1.00 25.15 1577 CZ PHE **ATOM** 363 72.860 22.521 10.219 1.00 24.41 **ATOM** 1578 C PHE 363 73.597 18.385 13.075 1.00 27.45 **ATOM** 1579 O PHE 363 73.577 19.324 13.880 1.00 27.73 ATOM 1580 N TRP 364 72.616 17.489 12.983 1.00 25.89 **ATOM** 1581 CA TRP 364 71.401 17.592 13.800 1.00 25.85 **ATOM** 1582 CB TRP 364. 70.444 16.426 13.506 1.00 24.27 **ATOM** 1583 CG TRP 364 69.168 16.391 14.328 1.00 23.75 **ATOM** 1584 CD2 TRP 364 68.152 17.407 14.397 1.00 24.87 **ATOM** 1585 CE2 TRP 364 67.140 16.922 15.261 1.00 24.81 **ATOM** 1586 CE3 TRP 364 67.989 18.674 13.820 1.00 25.47 **ATOM** 1587 CD1 TRP 364 68.745 15.370 15.122 1.00 22.98 **ATOM** 1588 NE1 TRP 364 67.530 15.679 15.684 1.00 25.99 **ATOM** 1589 CZ2 TRP 364 65.987 17.661 15.560 1.00 25.14 1590 CZ3 TRP 364 **ATOM** 66.844 19.405 14.116 1.00 25.29 **ATOM** 1591 CH2 TRP 364 65.857 18.894 14.982 1.00 24.53 1592 C **ATOM** TRP 364 71.659 17.747 15.308 1.00 26.94 **ATOM** 1593 O TRP 364 71.202 18.721 15.904 1.00 27.16 1594 N PRO **ATOM** 365 72.382 16.796 15.944 1.00 27.60 **ATOM** 1595 CD PRO 365 72.912 15.522 15.411 1.00 27.55 **ATOM** 1596 CA PRO 365 72.655 16.915 17.387 1.00 25.90 **ATOM** 1597 CB PRO 365 73.565 15.717 17.668 1.00 26.00 **ATOM** 1598 CG PRO 365 73.136 14.705 16.658 1.00 28.32 **ATOM** 1599 C PRO 365 73.374 18.225 17.714 1.00 23.89 **ATOM** 1600 O PRO 365 73.088 18.861 18.725 1.00 23.81 **ATOM** 1601 N LYS 366 74.297 18.626 16.845 1.00 24.24 1602 CA LYS **ATOM** 366 75.058 19.862 17.027 1.00 26.24

ATOM 1603 CB LYS 366 76.144 19.982 15.963 1.00 27.44 1604 CG LYS ATOM 366 77.310 19.022 16.138 1.00 28.76 **ATOM** 1605 CD LYS 366 78.254 19.171 14.975 1.00 30.53 ATOM 1606 CE LYS 79.527 18.387 15.167 1.00 34.25 366 **ATOM** 1607 NZ LYS 366 80.388 18.463 13.947 1.00 37.89 1608 C LYS **ATOM** 366 74.181 21.107 16.993 1.00 26.73 **ATOM** 1609 O LYS 366 74.385 22.042 17.762 1.00 27.36 **ATOM** 1610 N LEU 367 73.216 21.124 16.086 1.00 27.98 ATOM 1611 CA LEU 72.308 22.256 15.967 1.00 27.87 367 ATOM 1612 CB LEU 71.559 22.192 14.632 1.00 27.29 367 ATOM 1613 CG LEU 70.613 23.356 14.318 1.00 27.25 367 71.334 24.707 14.510 1.00 22.90 ATOM 1614 CD1 LEU 367 1615 CD2 LEU 367 ATOM 70.081 23.189 12.896 1.00 24.54 **ATOM** 1616 C LEU 367 71.327 22.223 17.134 1.00 29.38 **ATOM** 1617 O LEU 367 70.993 23.249 17.716 1.00 31.09 ATOM 1618 N LEU 368 70.889 21.026 17.491 1.00 30.38 **ATOM** 1619 CA LEU 368 69.962 20.843 18.594 1.00 31.14 ATOM 1620 CB LEU 368 69.659 19.353 18.731 1.00 32.20 1621 CG LEU ATOM 368 68.247 18.852 19.014 1.00 33.52 1622 CD1 LEU 67.184 19.651 18.267 1.00 31.14 **ATOM** 368 ATOM 1623 CD2 LEU 368 68.210 17.379 18.632 1.00 33.99 **ATOM** 1624 C LEU 368 70.601 21.395 19.876 1.00 32.36 **ATOM** 1625 O LEU 368 69.917 21.963 20.730 1.00 32.58 1626 N **ATOM** MET 369 71.922 21.272 19.985 1.00 33.30 **ATOM** 1627 CA MET 369 72.641 21.771 21.149 1.00 34.04 **ATOM** 1628 CB MET 369 74.051 21.190 21.209 1.00 35.31 1629 CG MET **ATOM** 369 74.108 19.858 21.935 1.00 36.83 **ATOM** 1630 SD MET 369 75.312 18.728 21.235 1.00 43.07 **ATOM** 1631 CE MET 369 76.862 19.636 21.472 1.00 41.31 **ATOM** 1632 C **MET** 369 72.675 23.297 21.212 1.00 34.30 **ATOM** 1633 O **MET** 369 72.961 23.876 22.269 1.00 35.82 **ATOM** 1634 N LYS 370 72.368 23.949 20.091 1.00 32.14 **ATOM** 1635 CA LYS 370 72.325 25.405 20.044 1.00 29.17 **ATOM** 1636 CB LYS 370 72.394 25.904 18.608 1.00 28.18 1637 CG LYS 370 73.662 25.518 17.900 1.00 27.72 **ATOM** 74.866 25.969 18.679 1.00 28.10 **ATOM** 1638 CD LYS 370 76.127 25.650 17.930 1.00 27.79 **ATOM** 1639 CE LYS 370 **ATOM** 1640 NZ LYS 370 77.298 25.941 18.777 1.00 30.78 **ATOM** 1641 C LYS 370 71.033 25.875 20.705 1.00 29.27 70.950 26.999 21.200 1.00 29.43 **ATOM** 1642 O LYS 370 **ATOM** 1643 N VAL 371 70.018 25.014 20.714 1.00 29.40 ATOM 1644 CA VAL 371 68.756 25.358 21.358 1.00 29.90 **ATOM** 1645 CB VAL 371 67.687 24.237 21.218 1.00 28.75 **ATOM** 1646 CG1 VAL 371 66.463 24.561 22.064 1.00 27.12 **ATOM** 1647 CG2 VAL 371 67.275 24.080 19.762 1.00 29.23 **ATOM** 1648 C VAL 371 69.075 25.573 22.832 1.00 31.39 **ATOM** 1649 O VAL 371 68.543 26.481 23.462 1.00 31.20

ATOM 1650 N THR 372 69.971 24.743 23.366 1.00 31.39 **ATOM** 1651 CA THR 372 70.371 24.847 24.762 1.00 31.10 **ATOM** 1652 CB THR 372 71.282 23.664 25.170 1.00 31.59 ATOM 1653 OG1 THR 372 70.554 22.441 25.008 1.00 30.60 **ATOM** 1654 CG2 THR 372 71.720 23.795 26.625 1.00 30.14 **ATOM** 1655 C THR 372 71.071 26.186 24.994 1.00 30.76 ATOM-1656 O THR 372 70.711 26.935 25.910 1.00 31.45 **ATOM** 1657 N **ASP** 373 72.038 26.507 24.138 1.00 29.31 **ATOM** 1658 CA ASP 373 72.744 27.772 24.252 1.00 27.32 **ATOM** 1659 CB ASP 373 73.745 27.934 23.115 1.00 27.98 **ATOM** 1660 CG ASP 373 74.886 26.933 23.190 1.00 28.94 1661 OD1 ASP **ATOM** 373 75.043 26.259 24.225 1.00 31.01 **ATOM** 75.639 26.825 22.205 1.00 31.38 1662 OD2 ASP 373 **ATOM** 1663 C ASP 373 71.742 28.926 24.247 1.00 26.50 **ATOM** 1664 O **ASP** 373 71.872 29.861 25.040 1.00 27.35 **ATOM** LEU 70.711 28.826 23.412 1.00 24.17 1665 N 374 **ATOM** 1666 CA LEU 374 69.688 29.864 23.331 1.00 23.38 **ATOM** 1667 CB LEU 374 68.795 29.660 22.107 1.00 22.98 **ATOM** 1668 CG LEU 374 69.361 30.183 20.786 1.00 24.45 **ATOM** 1669 CD1 LEU 374 68.668 29.520 19.589 1.00 24.72 **ATOM** 1670 CD2 LEU 374 69.223 31.704 20.735 1.00 22.40 ATOM 1671 C LEU 374 68.839 29.964 24.589 1.00 24.31 **ATOM** 1672 O LEU 374 68.442 31.065 24.986 1.00 23.31 **ARG** ATOM 1673 N 375 68.543 28.826 25.211 1.00 25.32 **ATOM** 1674 CA ARG 375 67.748 28.821 26.438 1.00 27.76 **1675 CB ARG ATOM** 375 67.455 27.392 26.908 1.00 30.82 **ATOM** 1676 CG ARG 375 66.901 26.439 25.854 1.00 38.79 **ATOM** 1677 CD ARG 375 65.424 26.630 25.582 1.00 45.40 **ATOM** 1678 NE ARG 375 64.709 25.360 25.620 1.00 52.61 **ATOM** 1679 CZ ARG 375 63.800 24.967 24.726 1.00 56.89 **ATOM** 1680 NH1 ARG 375 63.473 25.732 23.694 1.00 58.27 **ATOM** 1681 NH2 ARG 375 63.201 23.793 24.855 1.00 58.46 **ATOM** 1682 C ARG 375 68.563 29.542 27.512 1.00 26.98 **ATOM** 1683 O **ARG** 375 68.025 30.336 28.282 1.00 26.18 **ATOM** 1684 N MET 376 69.862 29.255 27.551 1.00 26.80 1685 CA MET 376 **ATOM** 70.767 29.867 28.511 1.00 29.22 **ATOM** 1686 CB MET 376 72.172 29.270 28.379 1.00 33.70 **ATOM** 1687 CG MET 376 72.595 28.371 29.562 1.00 43.20 **ATOM** 1688 SD MET 376 73.320 29.260 31.011 1.00 52.38 **ATOM** 1689 CE MET 376 71.843 29.854 31.913 1.00 48.11 **ATOM** 1690 C **MET** 376 70.804 31.384 28.339 1.00 27.54 1691 O **ATOM MET** 376 70.792 32.126 29.323 1.00 26.96 **ATOM** 1692 N ILE 377 70.841 31.835 27.087 1.00 25.39 **ATOM** 1693 CA ILE 377 70.847 33.264 26.767 1.00 23.26 **ATOM** 1694 CB ILE 377 70.992 33.488 25.222 1.00 22.73 **ATOM** 1695 CG2 ILE 377 70.560 34.909 24.819 1.00 21.81 **ATOM** 1696 CG1 ILE 377 72.431 33.205 24.789 1.00 20.39

ATOM 1697 CD1 ILE 377 72.644 33.148 23.300 1.00 18.85 **ATOM** 1698 C ILE 377 69.558 33.900 27.309 1.00 22.91 **ATOM** 1699 O ILE 377 69.597 34.925 27.989 1.00 22.02 1700 N **ATOM** GLY 378 68.427 33.244 27.069 1.00 22.29 **ATOM** 1701 CA GLY 378 67.161 33.757 27.547 1.00 22.83 **ATOM** 1702 C GLY 378 67.111 33.815 29.063 1.00 25.60 **ATOM** 1703 O GLY 378 66.546 34.752 29.630 1.00 26.25 ATOM 1704 N ALA 379 67.691 32.804 29.713 1.00 26.88 ATOM 1705 CA ALA 379 67.744 32.707 31.175 1.00 27.19 **ATOM** 1706 CB ALA 379 68.322 31.358 31.590 1.00 26.97 **ATOM** .1707 C ALA 379 68.606 33.827 31.738 1.00 26.13 **ATOM** 1708 O ALA 379 68.174 34.580 32.601 1.00 26.46 **ATOM** 1709 N CYA 380 69.826 33.935 31.230 1.00 27.61 **ATOM** 1710 CA CYA 380 70.742 34.973 31.667 1.00 29.74 **ATOM** 1711 CB CYA 72.070 34.865 30.923 1.00 35.44 380 ATOM 1712 SG CYA 380 73.081 33.458 31.417 1.00 42.61 **ATOM** 1713 AS CYA 380 74.829 33.691 29.945 1.00 55.91 **ATOM** 1714 C CYA 380 70.142 36.349 31.446 1.00 29.07 **ATOM** 1715 O **CYA** 380 70.243 37.225 32.303 1.00 29.46 ATOM 1716 N HIS 381 69.494 36.538 30.304 1.00 28.29 **ATOM** 1717 CA HIS 381 68.885 37.824 30.002 1.00 26.84 **ATOM** 1718 CB HIS 381 68.384 37.880 28.557 1.00 23.13 **ATOM** 1719 CG HIS 381 67.597 39.113 28.259 1.00 19.84 ATOM 1720 CD2 HIS 381 67.993 40.365 27.931 1.00 18.68 **ATOM** 1721 ND1 HIS 381 66.229 39.169 28.403 1.00 19.47 **ATOM** 1722 CE1 HIS 381 65.817 40.407 28.190 1.00 18.64 **ATOM** 1723 NE2 HIS 381 66.868 41.149 27.900 1.00 18.29 **ATOM** 1724 C HIS 381 67.747 38.157 30.967 1.00 26.78 **ATOM** 1725 O HIS 381 67.560 39.314 31.337 1.00 26.39 ALA 382 ATOM 1726 N 66.964 37.158 31.347 1.00 27.78 **ATOM** 1727 CA ALA 382 65.867 37.395 32.269 1.00 29.45 ATOM 1728 CB ALA 382 65.077 36.125 32.471 1.00 29.51 **ATOM** 1729 C ALA 382 66.425 37.904 33.604 1.00 31.74 **ATOM** 1730 O **ALA** 382 65.932 38.882 34.159 1.00 32.60 **ATOM** 1731 N SER 383 67.483 37.262 34.093 1.00 33.02 383 **ATOM** 1732 CA SER 68.109 37.662 35.350 1.00 34.69 ATOM 1733 CB SER 383 69.212 36.677 35.733 1.00 36.18 **ATOM** 1734 OG SER 383 68.663 35.386 35.933 1.00 40.61 **ATOM** 1735 C SER 383 68.689 39.064 35.242 1.00 33.49 1736 O **ATOM** SER 383 68.526 39.889 36.146 1.00 34.28 **ATOM** 1737 N ARG 384 69.377 39.332 34.141 1.00 32.60 **ATOM** 1738 CA ARG 384 69.955 40.642 33.938 1.00 32.60 **ATOM** 1739 CB ARG 384 70.926 40.638 32.762 1.00 33.60 **ATOM** 1740 CG ARG 384 71.429 42.013 32.409 1.00 36.33 1741 CD ARG 384 **ATOM** 72.875 41.975 31.993 1.00 39.62 **ATOM** 1742 NE ARG 384 73.760 42.260 33.114 1.00 41.76 74.587 43.301 33.179 1.00 41.92 **ATOM** 1743 CZ ARG 384

ATOM		74.670 44.182 32.191 1.00 40.66	
ATOM		75.319 43.471 34.260 1.00 44.88	••
ATOM			
ATOM	1751 CG PHE 385		
ATOM			
ATOM		63.281 42.580 32.689 1.00 25.01	
ATOM		· · ·	
ATOM			
ATOM	1756 CZ PHE 385		
ATOM	1757 C PHE 385	-	
ATOM	1758 O PHE 385	65.887 43.816 34.613 1.00 27.90	
ATOM	1759 N LEU 386	65.972 41.658 35.231 1.00 31.19	
ATOM		65.465 41.929 36.577 1.00 33.22	
ATOM	1761 CB LEU 386		
ATOM	1762 C LEU 386		
ATOM	1763 O LEU 386	65.874 43.907 37.855 1.00 32.93	
ATOM	1764 N HIS 387	67.673 42.760 37.158 1.00 34.80	
ATOM	1765 CA HIS 387		
ATOM	1766 CB HIS 387		
ATOM	1767 CG HIS 387	70.206 41.832 38.456 1.00 39.14	
ATOM	1768 CD2 HIS 387	69.307 41.080 39.144 1.00 39.28	
ATOM	1769 ND1 HIS 387	71.408 41.161 38.543 1.00 40.97	
ATOM	1770 CE1 HIS 387	71.241 40.055 39.245 1.00 41.57	
ATOM	1771 NE2 HIS 387	69.980 39.984 39.618 1.00 41.45	
ATOM	1772 C HIS 387		
ATOM	1773 O HIS 387		
ATOM	1774 N MET 388	•	÷
ATOM		68.398 46.455 35.168 1.00 46.28	
	1776 CB MET 388	68.170 46.286 33.665 1.00 43.30	
ATOM	1777 CG MET 388		
ATOM	1778 SD MET 388		
ATOM	1779 CE MET 388	68.208 44.370 30.709 1.00 42.36	
ATOM	1780 C MET 388	67.256 47.289 35.737 1.00 50.25	
ATOM	1781 O MET 388	67.363 48.506 35.886 1.00 49.79	
ATOM	1782 N LYS 389		ALTA
ATOM	1783 CA LYS 389	64.983 47.274 36.633 1.00 56.15	ALTA
ATOM	1784 CB LYS 389	63.770 46.334 36.565 1.00 56.87	ALTA
ATOM	1785 CG LYS 389	63.227 46.087 35.161 1.00 57.76	ALTA
ATOM	1786 CD LYS 389	62.029 45.156 35.212 1.00 55.98	ALTA
ATOM	1787 CE LYS 389	62.426 43.796 35.778 1.00 55.48	
ATOM	1788 NZ LYS 389	61.267 43.040 36.311 1.00 55.55	ALTA
ATOM	1789 C LYS 389	65.177 47.767 38.064 1.00 56.69	ALTA
ATOM	1790 O LYS 389	64.623 48.814 38.453 1.00 58.54	ALTA

ATOM 1791 N VAL 390 65.955 47.038 38.839 1.00 55.21 **ATOM** 1792 CA VAL 390 66.225 47.386 40.236 1.00 51.78 **ATOM** 1793 CB VAL 390 66.999 46.231 40.985 1.00 50.07 **ATOM** 1794 CG1 VAL 390 67.648 46.726 42.263 1.00 49.74 **ATOM** 1795 CG2 VAL 390 66.037 45.093 41.317 1.00 49.06 **ATOM** 1796 C VAL 390 67.053 48.681 40.227 1.00 49.38 **ATOM** 1797 O VAL 390 66.785 49.605 40.992 1.00 48.71 **ATOM** 1798 N **GLU** 391 67.974 48.778 39.272 1.00 46.71 **ATOM** 1799 CA GLU 391 68.866 49.919 39.142 1.00 44.88 **ATOM** 1800 CB GLU 391 70.156 49.488 38.438 1.00 45.24 1801 CG GLU ATOM 391 70.793 48.207 38.997 1.00 47.65 **ATOM** 1802 CD GLU 391 71.461 48.388 40.358 1.00 50.29 **ATOM** 1803 OE1 GLU 391 71.141 49.373 41.063 1.00 50.68 **ATOM** 1804 OE2 GLU 391 72.310 47.535 40.718 1.00 50.85 **ATOM** 1805 C 68.324 51.174 38.458 1.00 45.28 GLU 391 **ATOM** 1806 O GLU 391 68.568 52.286 38.940 1.00 46,46 **ATOM** 1807 N CYA 392 67.568 51.024 37.372 1.00 43.33 **ATOM** 1808 CA CYA 392 67.071 52.192 36.643 1.00 42.28 ATOM 1809 CB CYA 392 67.519 52.096 35.197 1.00 42.45 **ATOM** 1810 SG CYA 392 69.280 52.182 35.127 1.00 43.69 **ATOM** 1811 AS CYA 392 69.908 51.044 33.336 1.00 48.17 **ATOM** 1812 C CYA 392 65.589 52.493 36.709 1.00 42.51 **ATOM** 1813 O CYA 392 64.792 51.634 37.070 1.00 43.30 ATOM 1814 N PRO 393 65.205 53.752 36.418 1.00 42.13 **ATOM** 1815 CD PRO 393 66.109 54.899 36.199 1.00 40.54 **ATOM** 1816 CA PRO 393 63.794 54.182 36.441 1.00 42.26 **ATOM** 1817 CB PRO 393 63.896 55.710 36.365 1.00 41.47 **ATOM** 1818 CG PRO 65.189 55.938 35.614 1.00 41.10 393 **ATOM** 1819 C PRO 393 62.954 53.606 35.281 1.00 43.20 **ATOM** 1820 O **PRO** 393 63.463 53.452 34.163 1.00 42.61 1821 N **ATOM** THR 394 61.686 53.305 35.559 1.00 43.70 ATOM 1822 CA THR 394 60.764 52.755 34.564 1.00 45.50 **ATOM** 1823 CB THR 394 59.340 52.609 35.129 1.00 47.20 **ATOM** 1824 OG1 THR 394 59.304 53.139 36.464 1.00 50.57 **ATOM** 1825 CG2 THR 394 58.878 51.150 35.137 1.00 47.99 **ATOM** 1826 C THR 394 60.682 53.583 33.283 1.00 44.58 **ATOM** 1827 O THR 394 60.409 53.054 32.215 1.00 46.36 1828 N GLU 395 **ATOM** 60.899 54.888 33.396 1.00 42.88 ATOM 1829 CA GLU 395 60.842 55.790 32.246 1.00 40.54 **ATOM** 1830 CB GLU 395 61.096 57.234 32.699 1.00 40.69 **ATOM** 1831 C GLU 395 61.799 55.421 31.098 1.00 38.51 **ATOM** 1832 O GLU 395 61.628 55.877 29.968 1.00 39.41 **ATOM** 1833 N LEU 396 62.828 54.640 31.402 1.00 35.60 **ATOM** 1834 CA LEU 396 63.795 54.220 30.386 1.00 33.11 **ATOM** 1835 CB LEU 396 65.169 54.003 31.027 1.00 33.60 **ATOM** 1836 CG LEU 396 65.831 55.230 31.660 1.00 34.54 **ATOM** 1837 CD1 LEU 396 67.160 54.835 32.282 1.00 32.83

ATOM 1838 CD2 LEU 396 66.026 56.308 30.599 1.00 35.71 **ATOM** 1839 C LEU 396 63.388 52.940 29.660 1.00 30.95 **ATOM** 1840 O LEU 396 63.950 52.605 28.624 1.00 30.90 ATOM 1841 N PHE 397 62.422 52.227 30.223 1.00 30.18 **ATOM** 1842 CA PHE 397 61.961 50.970 29.654 1.00 28.80 1843 CB PHE **ATOM** 397 61.712 49.946 30.777 1.00 28.10 1844 CG PHE 397 ATOM 62.938 49.604 31.592 1.00 28.96 ATOM 1845 CD1 PHE 397 63.403 50.472 32.591 1.00 28.39 ATOM 1846 CD2 PHE 397 63.636 48.422 31.359 1.00 26.28 **ATOM** 1847 CE1 PHE 397 64.546 50.166 33.337 1.00 28.44 **ATOM** 1848 CE2 PHE 397 64.784 48.107 32.103 1.00 29.21 **ATOM** 1849 CZ PHE 397 65.240 48.984 33.096 1.00 27.37 1850 C ATOM PHE 397 60.683 51.093 28.836 1.00 27.54 **ATOM** 1851 O PHE 397 59.630 51.431 29.370 1.00 26.96 **ATOM** 1852 N PRO 398 60.753 50.836 27.501 1.00 27.41 398 **ATOM** 1853 CD PRO 61.968 50.600 26.686 1.00 25.42 **ATOM** 1854 CA PRO 398 59.560 50.920 26.654 1.00 25.90 60.068 50.383 25.320 1.00 25.26 **ATOM** 1855 CB PRO 398 **ATOM** 1856 CG PRO 398 61.490 50.893 25.290 1.00 23.99 **ATOM** 1857 C PRO 398 58.494 49.995 27.272 1.00 25.86 **ATOM** 1858 O PRO 398 58.839 48.962 27.843 1.00 25.82 1859 N PRO 399 ATOM 57.197 50.355 27.175 1.00 25.52 **ATOM** 1860 CD PRO 399 56.627 51.576 26.578 1.00 25.49 **ATOM** 1861 CA PRO 399 56.145 49.510 27.754 1.00 25.42 **ATOM** 1862 CB PRO 399 54.861 50.181 27.273 1.00 26.23 ATOM 1863 CG PRO 399 55.237 51.609 27.156 1.00 25.25 **ATOM** 1864 C PRO 399 56.198 48.043 27.317 1.00 26.08 **ATOM** 1865 O PRO 399 56.132 47.131 28.159 1.00 25.45 **ATOM** 1866 N LEU 400 56.350 47.810 26.019 1.00 25.57 56.406 46.440 25.509 1.00 26.27 ATOM 1867 CA LEU 400 **ATOM** 1868 CB LEU 400 56.404 46.418 23.980 1.00 25.03 400 ATOM 1869 CG LEU 56.117 45.042 23.363 1.00 24.51 400 **ATOM** 1870 CD1 LEU 54.757 44.530 23.806 1.00 23.22 **ATOM** 1871 CD2 LEU 400 56.173 45.149 21.862 1.00 23.70 **ATOM** 1872 C LEU 400 57.602 45.657 26.067 1.00 27.06 **ATOM** 1873 O LEU 400 57.484 44.465 26.363 1.00 27.41 **ATOM** 1874 N PHE 401 58.736 46.339 26.231 1.00 27.16 **ATOM** 1875 CA PHE 401 59.966 45.754 26.779 1.00 27.06 **ATOM** 1876 CB PHE 401 61.047 46.833 26.802 1.00 26.60 1877 CG PHE 401 **ATOM** 62.408 46.351 27.217 1.00 28.08 62.918 45.138 26.747 1.00 27.45 **ATOM** 1878 CD1 PHE 401 **ATOM** 1879 CD2 PHE 401 63.223 47.165 28.013 1.00 27.48 **ATOM** 1880 CE1 PHE 401 64.220 44.746 27.055 1.00 26.95 **ATOM** 1881 CE2 PHE 401 64.523 46.786 28.327 1.00 27.97 1882 CZ PHE 401 **ATOM** 65.028 45.575 27.846 1.00 28.46 **ATOM** 1883 C PHE 401 59.690 45.247 28.205 1.00 27.62 401 **ATOM** 1884 O PHE 60.046 44.125 28.570 1.00 26.24

ATOM	1885 N LEU 402	59.036 46.082 29.002 1.00 28.75	
ATOM	1886 CA LEU 402	58.692 45.719 30.366 1.00 29.58	••
ATOM	1887 CB LEU 402	58.064 46.910 31.088 1.00 30.04	
ATOM	1888 CG LEU 402	59.025 47.974 31.594 1.00 30.14	
ATOM	1889 CD1 LEU 402	58.270 49.263 31.880 1.00 29.61	
ATOM	1890 CD2 LEU 402	59.734 47.438 32.827 1.00 27.99	•
ATOM	1891 C LEU 402	57.693 44.583 30.368 1.00 30.10	
ATOM	1892 O LEU 402	57.836 43.631 31.121 1.00 29.78	
ATOM	1893 N GLU 403	56.688 44.683 29.510 1.00 30,49	٠.
ATOM	1894 CA GLU 403	55.646 43.671 29.453 1.00 32.60	
ATOM	1895 CB GLU 403	54.562 44.094 28.469 1.00 37.01	
ATOM	1896 CG GLU 403	53.329 43.218 28.520 1.00 44.01	
ATOM	1897 CD GLU 403	52.263 43.632 27.523 1.00 48.50	
ATOM	1898 OE1 GLU 403	52.516 44.525 26.677 1.00 49.66	
ATOM	1899 OE2 GLU 403	51.157 43.050 27.594 1.00 53.06	
ATOM	1900 C GLU 403	56.083 42.237 29.151 1.00 32.03	
ATOM	1901 O GLU 403	55.627 41.304 29.816 1.00 32.58	
ATOM	1902 N VAL 404	56.955 42.078 28.159 0.50 31.51	ALTA
ATOM	1903 CA VAL 404	57.450 40.765 27.739 0.50 30.96	ALTA
ATOM	1904 CB VAL 404	58.108 40.849 26.333 0.50 30.32	ALTA
ATOM	1905 CG1 VAL 404	58.616 39.489 25.889 0.50 28.72	ALTA
ATOM	1906 CG2 VAL 404	57.115 41.388 25.328 0.50 31.67	ALTA
ATOM	1907 C VAL 404	58.465 40.149 28.696 0.50 30.45	ALTA
ATOM	1908 O VAL 404	58.549 38.926 28.822 0.50 30.10	ALTA
ATOM	1909 N PHE 405	59.224 41.002 29.369 1.00 30.16	
ATOM	1910 CA PHE 405	60.266 40.549 30.263 1.00 30.65	
ATOM	1911 CB PHE 405	61.577 41.221 29.863 1.00 28.92	
ATOM	1912 CG PHE 405	62.062 40.834 28.493 1.00 26.31	
ATOM	1913 CD1 PHE 405	62.342 41.804 27.543 1.00 25.72	
ATOM ATOM	1914 CD2 PHE 405 1915 CE1 PHE 405	62.269 39.500 28.166 1.00 25.92	
ATOM	1915 CE1 PHE 405 1916 CE2 PHE 405	62.827 41.456 26.278 1.00 26.78 62.752 39.139 26.910 1.00 25.39	
ATOM	1917 CZ PHE 405	63.034 40.122 25.962 1.00 24.39	
ATOM		60.011 40.674 31.771 1.00 32.10	
ATOM	1919 O PHE 405	60.903 40.237 32.533 1.00 33.88	
ATOM	1920 OXT PHE 405	58.936 41.169 32.188 1.00 34.95	
ATOM	1 O1 HOH 501	67.542 37.066 11.311 1.00 26.83	
ATOM	3 O1 HOH 502	68.713 41.227 12.821 1.00 23.42	
ATOM	2 O1 HOH 503	64.446 40.325 12.123 1.00 22.84	
ATOM	4 O1 HOH 504	62.236 39.752 15.941 1.00 17.97	
ATOM	5 O1 HOH 505	48.732 20.137 5.515 1.00 50.48	
ATOM	6 O1 HOH 506	47.365 21.522 3.716 1.00 53.40	
ATOM	7 O1 HOH 507	50.211 23.203 7.900 1.00 32.66	
ATOM	8 O1 HOH 508	51.043 20.258 8.253 1.00 21.81	
ATOM	9 O1 HOH 509	48.225 18.176 7.905 1.00 38.96	
ATOM		49.569 20.871 11.586 1.00 32.97	
ATOM	11 O1 HOH 511	53.732 17.159 10.856 1.00 47.20	
			•

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ATOM	12 O1 HOH	512	56.201	16.223	12.164	1.00 18.50
ATOM	13 O1 HOH	513	56.653	12.298	10.528	1.00 27.71
ATOM	14 O1 HOH	514	58.661	10.694	9.014	1.00 46.73
ATOM	15 O1 HOH	515	62.950	10.692	11.952	1.00 43.05
ATOM	16 O1 HOH	516	66.411	11.552	10.897	1.00 37.36
ATOM	17 OF HOH	517	68.949	13.188	12.029	1.00 39.28
ATOM	18 O1 HOH	518	71.997	15.171	8.362	1.00 49.69
ATOM	19 O1 HOH	519	71.946	17.928	6.743	1.00 24.50
ATOM	20 O1 HOH	520	75.117	15.684	9.377	1.00 35.98
ATOM	21 O1 HOH	521	76.677	12.815	10.294	1.00 49.33
ATOM	22 O1 HOH	522	81.421	15.415	15.139	1.00 46.74
ATOM	23 O1 HOH	523	78.784	21.696	17.564	1.00 49.01
ATOM	24 O1 HOH	524	79.954	24.822	17.152	1.00 42.91
ATOM	25 O1 HOH	525	82.199	30.253	18.821	1.00 40.27
ATOM	26 O1 HOH	526	82.862	33.444	21.988	1.00 46.81
ATOM	27 O1 HOH	527	76.608	30.793	23.452	1.00 46.22
ATOM	28 O1 HOH	528	74.726	30.483	25.469	1.00 43.76
ATOM	29 O1 HOH	529		28.762	20.900	1.00 33.67
ATOM	30 O1 HOH	530		33.279	12.269	1.00 25.26
ATOM	31 O1 HOH	531		34.447	10.087	1.00 37.04
ATOM	32 O1 HOH	532	74.054	29.941		1.00 26.86
ATOM	33 O1 HOH	533	69.544	32.658		1.00 40.34
ATOM	34 O1 HOH	534		33.618		1.00 20.63
ATOM	35 O1 HOH	535	68.073	35.828		1.00 23.99
ATOM	36 O1 HOH	536	61.865	45.643		1.00 40.43
ATOM	37 O1 HOH	537	63.662	46.881	15.670	1.00 28.04
ATOM	38 O1 HOH	538	63.391	49.310	13.883	1.00 39.59
ATOM	39 O1 HOH	539	63.491	50.570	10.631	1.00 52.34
ATOM	40 O1 HOH	540	64.592	46.849	10.299	1.00 26.63
ATOM	41 O1 HOH	541	55.575	41.632	10.980	1.00 38.06
ATOM	42 O1 HOH	542	51.631	42.062	17.343	1.00 45.99
ATOM	43 O1 HOH	543	52.755	43.156	20.209	1.00 34.17
ATOM	44 O1 HOH	544	57.061	49.627	24.004	1.00 24.09
ATOM	45 O1 HOH	545	61.040	50.561	21.351	1.00 30.91
ATOM	46 O1 HOH	546	68.533	53.616	18.390	1.00 30.91
ATOM	47 O1 HOH	547	63.371	58.813	29.014	1.00 59.25
ATOM		548	57.934	52.905	31.175	1.00 40.12
ATOM	49 O1 HOH	549	62.364	50.496	37.543 1	1.00 52.28
ATOM	50 O1 HOH	550	62.256	19.704	40.891	1.00 54.18
ATOM	51 O1 HOH	551	61.994	46.430	40.384	1.00 43.84
ATOM	52 O1 HOH	552	63.675	14.459	39.268	1.00 44.73
ATOM	53 O1 HOH	553	58.405 4	13.920	33.936 1	1.00 42.88
ATOM	54 O1 HOH	554	62.863	39.071	34.046 1	.00 45.07
ATOM	55 O1 HOH	555	64.426 3	36.925	28.676 1	.00 25.36
ATOM		556				.00 21.14
ATOM		557	63.684 3			.00 33.03
ATOM		558		29.906		.00 57.37
		-		= •		- -

ATOM	59	0	нон 1	559	62.353	3 27.540	24.855	1.00 39.63
ATOM	60	O 1	HOH	560	62.814	28.785		
ATOM	61	O 1	HOH	561	65.531	30.642	28.821	1.00 54.44
ATOM	62	O1	HOH	562	63.423	24.645	32.964	1.00 50.75
ATOM	63	OI	НОН	563	64.697	21.149		1.00 51.41
ATOM	64	01	НОН	564	67.100	23.370	26.900	1.00 52.36
ATOM	65	01	НОН	565	65.582	20.422	23.303	1.00 40.32
ATOM	66	01	HOH	566	61.577	18.167	23.386	1.00 65.08
ATOM	67	01	HOH	567	61.022	22.649	25.573	1.00 48.85
ATOM	68	01	HOH	568	57.919	21.446	25.147	1.00 43.39
ATOM	69	01	HOH	569	59.435	20.179	28.543	1.00 51.41
ATOM	70	O 1	HOH	570	53.860	23.216	30.984	1.00 50.28
ATOM	71	01		571	52.825	24.880	32.696	1.00 43.96
ATOM	72	01	HOH	572	48.228	29.683	30.486	1.00 44.51
ATOM	73	01	HOH	573	48.925	34.467	30.521	1.00 36.28
ATOM	74	O 1	HOH	574	50.766	40.547	29.178	1.00 51.45
ATOM	75	O 1	HOH	575	57.058	32.490	30.420	1.00 31.03
ATOM	76	O 1	HOH	576	58.075	29.544	24.664	1.00 19.54
ATOM	77	01	HOH	577	47.451	19.292	28.703	1.00 33.04
ATOM	78	O 1	HOH	<i>5</i> 78	53.120	15.471	17.478	1.00 35.68
ATOM	79	01	HOH	579	55.101	14.146	16.095	1.00 50.46
ATOM	80	01	HOH	580	53.726	14.016		1.00 41.44
ATOM	81	01	НОН	581	57.223	13.820		1.00 48.31
ATOM	82	01	HOH	582	61.169	15.688		1.00 17.60
ATOM	83	01	HOH	583	67.411	16.019		1.00 23.93
ATOM	84	01	HOH	584	67.033	17.221		1.00 26.21
ATOM	85	01	HOH	585	69.893	19.520		1.00 59.67
ATOM	86	01	HOH	586	68.489	22.464		1.00 37.85
ATOM ATOM	87 88	01	HOH	587 599	65.794	23.354		1.00 27.38
ATOM	89	O1 O1	HOH HOH	588 589	67.550	26.810		1.00 37.18
ATOM		01	НОН	590	64.646 67.215	28.208 31.103		1.00 36.74
ATOM		01	НОН	591	64.164	35.667		1.00 30.29
ATOM		01	HOH	592		37.518		1.00 39.72 1.00 48.48
ATOM		01	НОН	593	68.105	36.898		1.00 48.48
ATOM		01	НОН	594		37.485		1.00 38.00
ATOM		01	НОН	595		36.068		1.00 57.29
ATOM			НОН	596		34.676		1.00 30.10
ATOM		01	НОН	597		31.465		1.00 42.32
ATOM		01	НОН	598		23.277		.00 28.98
ATOM			НОН	599		26.551		00 47.83
ATOM		01	НОН	600	46.411			1.00 53.46
ATOM		01	НОН	601	63.514			1.00 55.02
ATOM		01	НОН	602	67.943	11.792		1.00 61.21
ATOM		01	НОН	603	62.232	9.378		.00 35.65
ATOM		01	НОН	604		22.468		1.00 42.56
ATOM		01	НОН	605		28.967		1.00 50.64
				300	33.337	=0.707	J. 020 1	50.07

ATOM	.106	01	НОН	606	82.8	307 43.	437 17	.940	1.00 3	9.28
ATOM	107	01	HOH	607					1.00 4	
ATOM	108	01	HOH	608	80.2			.441	1.00 4	
ATOM	109	01	HOH	609	79.4		_	.165	1.00 3	
ATOM	110	01	НОН	610				.923	1.00 4	
ATOM	111	Oi	НОН	611	75.5			.384	1.00 2	
ATOM	112	01	НОН	612	77.1			575	1.00 3	
ATOM	113	01	HOH	613	73.5			926	1.00 2	
ATOM	114	01	HOH	614	75.9	55 56.5		863	1.00 4	
ATOM	115	01	HOH	615	79.9	15 59.		809	1.00 5	
ATOM	116	01	HOH	616	77.3	90 52.5			1.00 34	
ATOM	117	01	HOH	617	72.7	26 25.0		671	1.00 6	
ATOM	2038	С	ACY	701	52.60	54 40.1			1.00 46	
ATOM	2039	0	ACY	701	53.72	21 39.6	49 24.		1.00 47	
ATOM	2040	OX	T ACY	70	l 51.	652 40	.521 24			
ATOM	2041	CH	3 ACY	701		600 40.				
ATOM	2050	C1	T3	1	66.961	42.243	3 18.49	1 1.	00 22.3	4
ATOM	2051	C2	T3	1	68.748	43.593	3 23.01	5 1.	00 21.8	4
ATOM	2052	C3	T3	1	66.873	43.557	7 18.97	0 1.0	00 23.4	3
ATOM	2053	C4	T3	1	69.252	44.540	23.87	1 1.0	00 22.3	1
ATOM	2054	C5	T3	1	67.638	43.989	20.01	1 1.0	00 24.8	3
ATOM	2055	C6	T3	1	68.851	44.553	25.17	8 1.0	00 25.1	6
ATOM	2056	C7	T3	1	68.541	43.108	20.63	2 1.0	00 24.6	5
ATOM	2057	C8	T3	1	67.895	43.567	25.63	9 1.0	00 21.9	3
ATOM	2058		T3	1	68.665	41.792	20.18	3 1.0	00 25.0	9
ATOM	2059	C10		1	67.427	42.654	4 24.73	3 1.	00 23.6	6
ATOM	2060	C11		1	67.878	41.380	19.11	7 1.	00 23.1	2
ATOM	2061	C12		1		42.624	23.38	4 1.	00 19.6	7
ATOM	2062	C13		1	66.055	41.788			00 18.9	7
ATOM	2063	C15		1	66.721	40.956			00 19.3	2
ATOM		C17		1	65.901		15.05		00 19.0	
ATOM	2065			1	67.393					
ATOM	2066		•	1	69.483					
ATOM	2067				70.019					
ATOM			T3	1	68.131					
ATOM			T3	1	67.542					
ATOM			T3	1	69.259					
ATOM			T3	1	66.504					
MOTA	2072	O4	13	1	64.675	40.731	15.192	2 1.0	0 20.16	5
END										•

APPENDIX 7

TRBTRIAC.PDB

REMARK TR-beta Triac Full length numbering

REMARK refinement resolution: 100 - 2.9 A r = 0.273258 free r = 0.333794

REMARK wa = 5.78307

REMARK target = mlf cycles = 1 steps = 25

REMARK a = 68.72 b = 68.72 c = 130.092 alpha = 90 beta = 90 gamma = 120

REMARK ncs = none

REMARK initial B-factor correction: "none"

REMARK ALA 199 to ALA 201 from His-tag

REMARK

REMARK Four cacodylate-modified cysteines (CYA)

REMARK Cys294, Cys298, Cys388, Cys434

REMARK cacodylate modeled as single arsenic atom

REMARK

REMARK side chain of certain residues modeled as ALA due to poor density;

REMARK however, residue name reflects true residue for clarity

REMARK

REMARK amino acid sequence confirmed,

REMARK differing from that reported by Weinberger et. al.

REMARK in the following codons:

REMARK 243 Pro - Arg

REMARK 337 lle - Thr

REMARK 451 Leu - Phe

REMARK as reported by Sakurai et. al.

REMARK note also correction of initiation codon,

REMARK yielding a polypeptide of 461 amino acids

JRNL AUTH A.SAKURAI, A.NAKAI, L.J. DEGROOT

JRNL TITL STRUCTURAL ANALYSIS OF HUMAN THYROID HORMONE RECEPTOR

JRNL TITL2 BETA GENE

JRNL REF MOL.CELL.ENDO. V.71 1990

JRNL AUTH C.WEINBERGER, C.C.THOMPSON, R.LEBO, D.J. GRUOL, R.M. EVANS

JRNL TITL THE C-ERB-A GENE ENCODES A THYROID HORMONE RECEPTOR

JRNL REF NATURE V.324 6098 1986

ATOM	1 CB ALA 199	31.247 28.289 43.613 1.00 71.30	PROT
ATOM	2 C ALA 199	32.916 26.485 44.170 1.00 68.99	PROT
ATOM	3 O ALA 199	33.485 25.410 43.976 1.00 63.84	PROT
ATOM	4 N ALA 199	30.462 25.993 44.096 1.00 75.00	PROT
ATOM	5 CA ALA 199	31.571 26.795 43.497 1.00 73.24	PROT
ATOM	6 N ALA 200	33.419 27.432 44.958 1.00 73.81	PROT
ATOM	7 CA ALA 200	34.686 27.251 45.658 1.00 67.87	PROT
ATOM	8 CB ALA 200	35.182 28.583 46.203 1.00 62.83	PROT
ATOM	9 C ALA 200	34.539 26.239 46.791 1.00 63.23	PROT

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ATOM	10 O ALA 200	35.486 25.986 47.534 1.00 59.14	PROT
ATOM	11 N ALA 201	33.345 25.670 46.932 1.00 56.98	PROT
ATOM	12 CA ALA 201	33.117 24.664 47.957 1.00 51.46	PROT
ATOM	13 CB ALA 201	31.776 23.992 47.744 1.00 40.35	PROT
ATOM	14 C ALA 201	34.248 23.662 47.762 1.00 53.15	PROT
ATOM	15 O ALA 201	34.624 22.938 48.679 1.00 54.90	PROT
ATOM	16 N GLU 202	34.789 23.645 46.546 1.00 44.13	PROT
ATOM	17 CA GLU 202	35.891 22.767 46.190 1.00 37.47	PROT
ATOM	18 CB GLU 202	36.086 22.760 44.671 1.00 37.74	PROT
ATOM	19 CG GLU 202	37.060 21.702 44.173 1.00 57.14	PROT
ATOM	20 CD GLU 202	36.457 20.303 44.140 1.00 61.74	PROT
ATOM	21 OE1 GLU 202	35.211 20.175 44.133 1.00 63.81	PROT
ATOM	22 OE2 GLU 202	37.236 19.327 44.115 1.00 65.54	PROT
ATOM	23 C GLU 202	37.156 23.266 46.878 1.00 35.54	PROT
ATOM	24 O GLU 202	37.874 22.492 47.510 1.00 32.70	PROT
ATOM	25 N GLU 203	37.415 24.566 46.755 1.00 31.79	PROT
ATOM	26 CA GLU 203	38.588 25.188 47.366 1.00 33.63	PROT
ATOM	27 CB GLU 203	38.603 26.683 47.079 1.00 28.28	PROT
ATOM	28 C GLU 203	38.588 24.948 48.869 1.00 33.86	PROT
ATOM	29 O GLU 203	39.644 24.818 49.485 1.00 33.10	PROT
ATOM	30 N LEU 204	37.393 24.898 49.451 1.00 34.15	PROT
ATOM	31 CA LEU 204	37.244 24.650 50.876 1.00 33.22	PROT
ATOM	32 CB LEU 204	35.853 25.081 51.353 1.00 30.47	PROT
ATOM	33 CG LEU 204	35.567 25.083 52.862 1.00 23.17	PROT
ATOM	34 CD1 LEU 204	35.904 26.439 53.443 1.00 5.41	PROT
ATOM	35 CD2 LEU 204	34.106 24.748 53.111 1.00 12.70	PROT
ATOM	36 C LEU 204	37.424 23.156 51.100 1.00 40.17	PROT
ATOM	37 O LEU 204	38.219 22.736 51.951 1.00 45.33	PROT
ATOM	38 N GLN 205	36.682 22.360 50.329 1.00 43.86	PROT
ATOM	39 CA GLN 205	36.754 20.899 50.415 1.00 43.96	PROT
ATOM	40 CB GLN 205	36.089 20.261 49.184 1.00 45.56	PROT
ATOM	41 CG GLN 205	34.562 20.195 49.245 1.00 42.39	PROT
ATOM	42 CD GLN 205	34.022 18.775 49.159 1.00 46.79	PROT
ATOM	43 OE1 GLN 205	33.258 18.444 48.252 1.00 38.84	PROT
ATOM	44 NE2 GLN 205	34.412 17.932 50.109 1.00 37.95	PROT
ATOM	45 C GLN 205	38.224 20.482 50.483 1.00 42.39	PROT
ATOM	46 O GLN 205	38.630 19.702 51.355 1.00 36.27	PROT
ATOM	47 N LYS 206	39.014 21.015 49.553 1.00 42.37	PROT
ATOM	48 CA LYS 206	40.440 20.729 49.505 1.00 44.40	PROT
ATOM	49 CB LYS 206	41.110 21.531 48.385 1.00 38.73	PROT
ATOM	50 C LYS 206	41.024 21.118 50.853 1.00 42.36	PROT
ATOM	51 O LYS 206	41.550 20.271 51.570 1.00 46.93	PROT
ATOM	52 N SER 207	40.913 22.401 51.192 1.00 34.68	PROT
ATOM	53 CA SER 207	41.415 22.933 52.455 1.00 29.43	PROT
ATOM	54 CB SER 207	40.690 24.228 52.791 1.00 24.63	PROT
ATOM	55 OG SER 207	41.327 25.332 52.173 1.00 36.56	PROT

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ATOM	56 C SER 207	41.254 21.958 53.614 1.00 29.20	PROT
ATOM	57 O SER 207	42.223 21.623 54.293 1.00 31.01	PROT
ATOM	58 N ILE 208	40.028 21.504 53.841 1.00 22.55	PROT
ATOM	59 CA ILE 208	39.777 20.568 54.928 1.00 27.93	PROT
ATOM	60 CB ILE 208	38.267 20.216 55.027 1.00 39.85	PROT
ATOM	61 CG2 ILE 208	38.062 18.895 55.769 1.00 32.13	PROT
ATOM	62 CG1 ILE 208	37.528 21.340 55.753 1.00 37.63	PROT
ATOM	63 CD1 ILE 208	36.788 22.296 54.827 1.00 41.47	PROT
ATOM	64 C ILE 208	40.591 19.291 54.725 1.00 29.61	PROT
ATOM	65 O ILE 208	40.905 18.580 55.679 1.00 40.00	PROT
ATOM	66 N GLY 209	40.928 19.002 53.475 1.00 35.05	PROT
ATOM	67 CA GLY 209	41.698 17.809 53.181 1.00 31.94	PROT
ATOM	68 C GLY 209	40.826 16.695 52.643 1.00 28.66	PROT
ATOM	69 O GLY 209	41.257 15.553 52.532 1.00 19.46	PROT
ATOM	70 N HIS 210	39.586 17.021 52.313 1.00 20.47	PROT
ATOM	71 CA HIS 210	38.684 16.018 51.774 1.00 26.99	PROT
ATOM	72 CB HIS 210	37.240 16.451 52.012 1.00 37.16	PROT
ATOM	73 C HIS 210	38.959 15.806 50.266 1.00 27.75	PROT
ATOM	74 O HIS 210	39.328 16.741 49.550 1.00 34.08	PROT
ATOM	75 N LYS 211	38.807 14.566 49.805 1.00 16.50	PROT
ATOM	76 CA LYS 211	39.019 14.206 48.403 1.00 5.57	PROT
ATOM	77 CB LYS 211	39.932 12.981 48.295 1.00 5.67	PROT
ATOM	78 CG LYS 211	41.370 13.208 48.742 1.00 7.30	PROT
ATOM	79 CD LYS 211	41.873 14.594 48.347 1.00 14.34	PROT
ATOM	80 CE LYS 211	43.339 14.556 47.897 1.00 29.48	PROT
ATOM	81 NZ LYS 211	43.777 15.851 47.262 1.00 33.43	PROT
ATOM	82 C LYS 211	37.642 13.861 47.876 1.00 2.73	PROT
ATOM	83 O LYS 211	37.176 12.741 48.039 1.00 6.57	PROT
ATOM	84 N PRO 212	36.983 14.813 47.208 1.00 2.00	PROT
ATOM	85 CD PRO 212	37.472 16.156 46.846 1.00 10.43	PROT
ATOM	86 CA PRO 212	35.642 14.542 46.689 1.00 2.05	PROT
ATOM	87 CB PRO 212	35.088 15.928 46.341 1.00 10.09	PROT
ATOM	88 CG PRO 212	36.240 16.888 46.422 1.00 8.43	PROT
ATOM	89 C PRO 212	35.523 13.578 45.520 1.00 2.00	PROT
ATOM	90 O PRO 212	36.344 13.554 44:611 1.00 6.04	PROT
ATOM	91 N GLU 213	34.476 12.773 45.577 1.00 2.68	PROT
ATOM	92 CA GLU 213	34.181 11.817 44.542 1.00 6.81	PROT
ATOM	93 CB GLU 213	33.539 10.594 45.173 1.00 7.20	PROT
ATOM	94 CG GLU 213	34.222 10.232 46.462 1.00 15.33	PROT
ATOM	95 CD GLU 213 96 OE1 GLU 213	34.293 8.743 46.689 1.00 21.36	PROT
ATOM		33.334 8.051 46.290 1.00 29.32	PROT
ATOM	97 OE2 GLU 213	35.301 8.265 47.268 1.00 28.50	PROT
ATOM	98 C GLU 213	33.229 12.543 43.584 1.00 12.00	PROT
ATOM	99 O GLU 213	32.693 13.599 43.926 1.00 19.02 33.011 11.095 42.375 1.00 25.74	PROT
ATOM	100 N PRO 214	33.011 11.985 42.375 1.00 25.74	PROT
ATOM	101 CD PRO 214	33.592 10.692 41.973 1.00 28.98	PROT

ATOM	102 CA PRO 214	32.145 12.536 41.322 1.00 23.38	PROT
ATOM	103 CB PRO 214	32.180 11.476 40.232 1.00 18.01	PROT
ATOM	104 CG PRO 214	33.376 10.665 40.514 1.00 27.50	PROT
ATOM	105 C PRO 214	30.715 12.828 41.734 1.00 25.02	PROT
ATOM	106 O PRO 214	30.069 11.986 42.355 1.00 31.17	PROT
ATOM	107 N- THR 215	30.211 14.009 41.377 1.00 19.56	PROT
ATOM	108 CA THR 215	28.830 14.352 41.714 1.00 24.48	PROT
ATOM	109 CB THR 215	28.535 15.841 41.522 1.00 27.13	PROT
ATOM	110 OG1 THR 215	27.939 16.038 40.234 1.00 40.19	PROT
ATOM	111 CG2 THR 215	29.805 16.659 41.640 1.00 30.81	PROT
ATOM	112 C THR 215	27.899 13.562 40.805 1.00 22.14	PROT
ATOM	113 O THR 215	28.357 12.905 39.883 1.00 27.52	PROT
ATOM	114 N ASP 216	26.599 13.617 41.072 1.00 35.65	PROT
ATOM	115 CA ASP 216	25.631 12.890 40.258 1.00 41.16	PROT
ATOM	116 CB ASP 216	24.219 13.091 40.810 1.00 38.17	PROT
ATOM	117 C ASP 216	25.714 13.370 38.810 1.00 40.44	PROT
ATOM	118 O ASP 216	25.683 12.569 37.874 1.00 38.26	PROT
ATOM	119 N GLU 217	25.832 14.682 38.635 1.00 40.14	PROT
ATOM	120 CA GLU 217	25.932 15.275 37.305 1.00 38.89	PROT
ATOM	121 CB GLU 217	25.883 16.796 37.413 1.00 29.95	PROT
ATOM	122 C GLU 217	27.231 14.829 36.619 1.00 39.44	PROT
ATOM	123 O GLU 217	27.245 14.525 35.425 1.00 40.08	PROT
ATOM	124 N GLU 218	28.319 14.794 37.384 1.00 34.92	PROT
ATOM	125 CA GLU 218	29.615 14.370 36.871 1.00 23.70	PROT
ATOM	126 CB GLU 218	30.698 14.606 37.924 1.00 18.47	PROT
ATOM	127 CG GLU 218	30.990 16.067 38.198 1.00 15.66	PROT
ATOM	128 CD GLU 218	32.085 16.264 39.231 1.00 26.88	PROT
ATOM	129 OE1 GLU 218	32.164 15.458 40.191 1.00 25.07	PROT
ATOM	130 OE2 GLU 218	32.864 17.232 39.078 1.00 33.79	PROT
ATOM	131 C GLU 218	29.589 12.892 36.491 1.00 21.05	PROT
ATOM	132 O GLU 218	30.182 12.490 35.495 1.00 24.30	PROT
ATOM ATOM	133 N TRP 219 134 CA TRP 219	28.907 12.080 37.288 1.00 13.98	PROT
ATOM		28.829 10.660 37.000 1.00 17.30	PROT
ATOM	135 CB TRP 219 136 CG TRP 219	28.052 9.921 38.089 1.00 16.27	PROT
ATOM	130 CG TRP 219 137 CD2 TRP 219	28.890 9.520 39.277 1.00 31.14 29.984 8.585 39.296 1.00 36.40	PROT
ATOM	137 CD2 TRP 219 138 CE2 TRP 219	30.476 8.547 40.621 1.00 29.24	PROT
ATOM	139 CE3 TRP 219	30.595 7.781 38.323 1.00 41.61	PROT PROT
ATOM	140 CD1 TRP 219	28.771 9.988 40.551 1.00 28.69	PROT
ATOM	141 NE1 TRP 219	29.718 9.411 41.362 1.00 25.09	PROT
ATOM	141 KEI TRF 219	31.552 7.737 41.004 1.00 30.89	PROT
ATOM	142 CZ2 TRI 219	31.673 6.969 38.707 1.00 45.72	PROT
ATOM	144 CH2 TRP 219	32.137 6.958 40.038 1.00 35.17	PROT
ATOM	145 C TRP 219	28.125 10.500 35.660 1.00 20.83	PROT
ATOM	146 O TRP 219	28.467 9.616 34.865 1.00 31.36	PROT
ATOM	147 N GLU 220	27.143 11.364 35.412 1.00 30.53	PROT
	177 17 OLO 220	21.175 II.UU JU.J3	INI

ATOM	.148 CA GLU 220	26.400 11.323 34.159 1.00 33.95	PROT
ATOM	149 CB GLU 220	25.237 12.318 34.201 1.00 22.17	PROT
ATOM	150 C GLU 220	27.356 11.658 33.013 1.00 34.66	PROT
ATOM	151 O GLU 220	27.233 11.134 31.900 1.00 43.86	PROT
ATOM	152 N LEU 221	28.320 12.528 33.297 1.00 22.60	PROT
ATOM	153 CA LEU 221	29.305 12.926 32.304 1.00 17.18	PROT
ATOM	154 CB LEU 221	29.995 14.219 32.743 1.00 11.03	PROT
ATOM	155 CG LEU 221	31.078 14.824 31.850 1.00 5.17	PROT
ATOM	156 CD1 LEU 221	30.756 14.569 30.415 1.00 6.41	PROT
ATOM	157 CD2 LEU 221	31.181 16.305 32.092 1.00 10.65	PROT
ATOM	158 C LEU 221	30.344 11.817 32.122 1.00 22.25	PROT
ATOM	159 O LEU 221	30.759 11.521 31.002 1.00 18.99	PROT
ATOM	160 N ILE 222	30.754 11.198 33.228 1.00 20.74	PROT
ATOM	161 CA ILE 222	31.744 10.136 33.177 1.00 12.88	PROT
ATOM	162 CB ILE 222	32.115 9.662 34.587 1.00 12.96	PROT
ATOM	163 CG2 ILE 222	33.030 8.468 34.515 1.00 2.00	PROT
ATOM	164 CG1 ILE 222	32.811 10.796 35.332 1.00 16.50	PROT
ATOM	165 CD1 ILE 222	33.625 10.351 36.511 1.00 15.90	PROT
ATOM	166 C ILE 222	31.241 8.958 32.363 1.00 17.72	PROT
ATOM	167 O ILE 222	32.001 8.363 31.594 1.00 16.59	PROT
ATOM	168 N LYS 223	29.966 8.618 32.530 1.00 33.88	PROT
ATOM	169 CA LYS 223	29.371 7.503 31.795 1.00 39.02	PROT
ATOM	170 CB LYS 223	27.908 7.307 32.224 1.00 40.29	PROT
ATOM	171 C LYS 223	29.444 7.779 30.293 1.00 39.14	PROT
ATOM	172 O LYS 223	29.949 6.963 29.517 1.00 32.99	PROT
ATOM	173 N THR 224	28.936 8.942 29.897 1.00 27.19	PROT
ATOM	174 CA THR 224	28.929 9.363 28.498 1.00 25.75	PROT
ATOM	175 CB THR 224	28.440 10.817 28.407 1.00 22.51	PROT
ATOM	176 OG1 THR 224	27.018 10.837 28.568 1.00 35.46	PROT
ATOM	177 CG2 THR 224	28.799 11.436 27.083 1.00 15.53	PROT
ATOM	178 C THR 224	30.307 9.235 27.833 1.00 22.31	PROT
ATOM	179 O THR 224	30.480 8.517 26.843 1.00 27.13	PROT
ATOM	180 N VAL 225	31.287 9.936 28.386 1.00 17.87	PROT
ATOM	181 CA VAL 225	32.635 9.906 27.854 1.00 17.07	PROT
ATOM	182 CB VAL 225	33.559 10.759 28.720 1.00 16.86	PROT
ATOM	183 CG1 VAL 225	34.845 11.064 27.973 1.00 26.54	PROT
ATOM	184 CG2 VAL 225	32.854 12.057 29.075 1.00 24.46	PROT
ATOM	185 C VAL 225	33.169 8.486 27.793 1.00 16.11	PROT
ATOM	186 O VAL 225	33.683 8.042 26.763 1.00 12.75	PROT
ATOM	187 N THR 226	33.040 7.769 28.900 1.00 12.23	PROT
ATOM	188 CA THR 226	33.520 6.400 28.951 1.00 12.34	PROT
ATOM	189 CB THR 226	33.175 5.747 30.271 1.00 17.01	PROT
ATOM	190 OG1 THR 226	33.715 6.536 31.342 1.00 6.78	PROT
ATOM	191 CG2 THR 226	33.739 4.324 30.307 1.00 2.00	PROT
ATOM	192 C THR 226	32.909 5.581 27.837 1.00 14.82	PROT
ATOM	193 O THR 226	33.623 4.953 27.061 1.00 20.90	PROT

ATOM 194 N GLU 227 ATOM 195 CA GLU 227 ATOM 196 CB GLU 227 ATOM 197 C GLU 227 ATOM 198 O GLU 227 ATOM 199 N ALA 228 ATOM 199 N ALA 228 ATOM 200 CA ALA 228 ATOM 201 CB ALA 228 ATOM 201 CB ALA 228 ATOM 202 C ALA 228 ATOM 202 C ALA 228 ATOM 205 CA HIS 229 ATOM 206 CB HIS 229 ATOM 207 CG HIS 229 ATOM 208 CD2 HIS 229 ATOM 207 CG HIS 229 ATOM 208 CD2 HIS 229 ATOM 209 NDI HIS 229 ATOM 210 CEI HIS 229 ATOM 211 NEZ HIS 229 ATOM 212 C HIS 229 ATOM 213 O HIS 229 ATOM 215 CA VAL 230 ATOM 215 CA VAL 230 ATOM 216 CB VAL 230 ATOM 217 CGI VAL 230 ATOM 218 CG2 VAL 230 ATOM 217 CGI VAL 230 ATOM 218 CG2 VAL 230 ATOM 217 CGI VAL 230 ATOM 218 CG2 VAL 230 ATOM 217 CGI VAL 230 ATOM 220 C ALA 231 ATOM 221 C HIS 232 ATOM 222 CA ALA 231 ATOM 223 CB ALA 231 ATOM 224 C ALA 231 ATOM 225 CA RIN 232 ATOM 226 CB THR 232 ATOM 227 CA THR 232 ATOM 228 CB ALA 231 ATOM 229 CG ANN 233 ATOM 233 N ASN 233 ATOM 234 CA ASN 233 ATOM 235 CB ASN 233 ATOM 236 CG ASN 233 ATOM 237 CA SN 233 ATOM 237 CA SN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 237 CA SN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 239 C ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 238 CD ASN 233 ATOM 248 CG				
ATOM 196 CB GLU 227	ATOM	194 N GLU 227		PROT
ATOM 197 C GLU 227 31.556 5.173 25.386 1.00 21.74 PROT ATOM 198 O GLU 227 32.057 4.283 24.700 1.00 24.42 PROT ATOM 199 N. ALA 228 31.590 6.460 25.050 1.00 13.26 PROT ATOM 200 CA ALA 228 32.190 6.928 23.800 1.00 22.76 PROT ATOM 201 CB ALA 228 32.196 6.928 23.800 1.00 22.75 PROT ATOM 202 C ALA 228 33.584 6.358 23.538 1.00 19.19 PROT ATOM 203 O ALA 228 33.913 6.003 22.408 1.00 17.19 PROT ATOM 204 N HIS 229 34.408 6.290 24.573 1.00 20.11 PROT ATOM 205 CA HIS 229 35.741 5.756 24.389 1.00 18.68 PROT ATOM 206 CB HIS 229 35.541 5.756 24.389 1.00 18.68 PROT ATOM 207 CG HIS 229 37.894 5.201 25.586 1.00 2.00 PROT ATOM 207 CG HIS 229 38.800 5.517 24.582 1.00 3.78 PROT ATOM 209 NDI HIS 229 38.780 5.517 24.582 1.00 3.78 PROT ATOM 211 NEZ HIS 229 39.771 4.090 25.840 1.00 7.10 PROT ATOM 211 NEZ HIS 229 39.771 4.090 25.840 1.00 7.10 PROT ATOM 212 C HIS 229 33.4827 24.758 1.00 13.68 PROT ATOM 213 O HIS 229 36.127 3.950 22.866 1.00 22.42 PROT ATOM 216 CB VAL 230 34.827 2.086 24.468 1.00 33.80 PROT ATOM 216 CB VAL 230 34.827 2.086 24.468 1.00 33.80 PROT ATOM 217 CGI VAL 230 34.251 -0.106 25.515 1.00 33.80 PROT ATOM 218 CG2 VAL 230 34.224 1.781 23.100 1.00 33.11 PROT ATOM 220 CVAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 221 C ALA 231 33.170 2.507 22.746 1.00 36.22 PROT ATOM 222 CA ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 222 CA ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 222 CA ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 222 CA ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 222 CA ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 226 CB THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 231 C THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 231 C THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 232 CB ALA 231 33.445 2.501 20.303 1.00 35.94 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 4.71 PROT ATOM 231 C THR 232 35.335 5.321 19.238 1.00 4.71 PROT ATOM 230 CG2 THR 232 35.735 5.321 19.238 1.00 9.70				PROT
ATOM 198 O GLU 227 32.057 4.283 24.700 1.00 24.42 PROT ATOM 199 N. ALA 228 31.590 6.460 25.050 1.00 13.26 PROT ATOM 200 CA ALA 228 32.196 6.928 23.800 1.00 22.76 PROT ATOM 201 CB ALA 228 32.267 8.450 23.785 1.00 22.50 PROT ATOM 202 C ALA 228 33.584 6.358 23.538 1.00 19.19 PROT ATOM 203 O ALA 228 33.913 6.003 22.408 1.00 17.19 PROT ATOM 204 N HIS 229 34.408 6.290 24.573 1.00 20.11 PROT ATOM 205 CA HIS 229 35.741 5.756 24.389 1.00 18.68 PROT ATOM 206 CB HIS 229 36.537 5.819 25.686 1.00 10.37 PROT ATOM 207 CG HIS 229 38.780 4.299 26.376 1.00 7.61 PROT ATOM 208 CD2 HIS 229 38.780 4.299 26.376 1.00 7.61 PROT ATOM 210 CE1 HIS 229 39.900 4.837 24.758 1.00 15.67 PROT ATOM 211 NE2 HIS 229 39.711 4.090 25.840 1.00 7.10 PROT ATOM 211 NE2 HIS 229 35.637 4.316 23.940 1.00 21.45 PROT ATOM 213 O HIS 229 33.4893 3.505 24.762 1.00 21.45 PROT ATOM 216 CB VAL 230 34.983 3.505 24.762 1.00 21.45 PROT ATOM 217 CG1 VAL 230 34.281 1.985 26.896 1.00 33.80 PROT ATOM 217 CG1 VAL 230 34.281 1.985 26.896 1.00 33.11 PROT ATOM 218 CG2 VAL 230 34.228 1.985 26.896 1.00 33.11 PROT ATOM 219 C VAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 220 O VAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 221 N ALA 231 33.170 2.507 22.786 1.00 30.31 PROT ATOM 221 C ALA 231 33.425 1.985 26.896 1.00 26.54 PROT ATOM 222 CA ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 224 C ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 226 C THR 232 35.335 5.321 19.238 1.00 15.54 PROT ATOM 227 CA THR 232 35.335 5.321 19.238 1.00 15.54 PROT ATOM 227 CA THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 227 CA THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 231 C THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 231 C THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 232 CB ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 230 CG2 THR 232 35.335 5.321 19.238 1.00 2.00 PROT ATOM 230 CG2 THR 232 35.335 2.0523 1.00 28				PROT
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ATOM 216 CB VAL 230 33.960 1.388 25.528 1.00 33.11 PROT ATOM 217 CG1 VAL 230 34.251 -0.106 25.515 1.00 33.80 PROT ATOM 218 CG2 VAL 230 34.228 1.985 26.896 1.00 26.54 PROT ATOM 219 C VAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 220 O VAL 230 34.703 0.897 22.385 1.00 40.80 PROT ATOM 221 N ALA 231 33.170 2.507 22.746 1.00 36.22 PROT ATOM 222 CA ALA 231 32.497 2.298 21.471 1.00 36.24 PROT ATOM 223 CB ALA 231 31.318 3.255 21.343 1.00 18.90 PROT ATOM 224 C ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 225 O ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 226 N THR 232 34.380 3.434 20.474 1.00 23.74 PROT ATOM 227 CA THR 232 35.329 3.789 19.432 1.00 15.54 PROT ATOM 228 CB THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 230 CG2 THR 232 35.733 5.949 20.460 1.00 16.73 PROT ATOM 231 C THR 232 35.733 5.949 20.460 1.00 16.73 PROT ATOM 231 C THR 232 36.758 3.309 19.670 1.00 19.86 PROT ATOM 232 O THR 232 37.695 3.854 19.094 1.00 15.31 PROT ATOM 233 N ASN 233 36.938 2.305 20.523 1.00 28.26 PROT ATOM 234 CA ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 235 CB ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 236 CG ASN 233 38.845 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 38.845 1.343 22.234 1.00 47.14 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 237 OD1 ASN 233 40.663 2.303 22.128 1.00 60.36 PROT ATOM 238 ND2 ASN 233 40.645 1.296 24.045 1.00 48.67 PROT	ATOM	214 N VAL 230	34.983 3.505 24.762 1.00 21.64	PROT
ATOM 217 CG1 VAL 230 34.251 -0.106 25.515 1.00 33.80 PROT ATOM 218 CG2 VAL 230 34.228 1.985 26.896 1.00 26.54 PROT ATOM 219 C VAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 220 O VAL 230 34.703 0.897 22.385 1.00 40.80 PROT ATOM 221 N ALA 231 33.170 2.507 22.746 1.00 36.22 PROT ATOM 222 CA ALA 231 32.497 2.298 21.471 1.00 36.24 PROT ATOM 223 CB ALA 231 31.318 3.255 21.343 1.00 18.90 PROT ATOM 224 C ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 225 O ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 226 N THR 232 34.380 3.434 20.474 1.00 23.74 PROT ATOM 227 CA THR 232 35.329 3.789 19.432 1.00 15.54 PROT ATOM 228 CB THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 229 OG1 THR 232 35.733 5.949 20.460 1.00 16.73 PROT ATOM 230 CG2 THR 232 33.942 5.828 18.891 1.00 2.00 PROT ATOM 231 C THR 232 36.758 3.309 19.670 1.00 19.86 PROT ATOM 232 O THR 232 37.695 3.854 19.094 1.00 15.31 PROT ATOM 233 N ASN 233 36.938 2.305 20.523 1.00 28.26 PROT ATOM 234 CA ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 235 CB ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 236 CG ASN 233 38.435 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 38.804 1.689 22.801 1.00 54.02 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 237 OD1 ASN 233 40.645 1.296 24.045 1.00 48.67 PROT	ATOM	215 CA VAL 230	34.827 2.086 24.468 1.00 33.80	PROT
ATOM 218 CG2 VAL 230 34.228 1.985 26.896 1.00 26.54 PROT ATOM 219 C VAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 220 O VAL 230 34.703 0.897 22.385 1.00 40.80 PROT ATOM 221 N ALA 231 33.170 2.507 22.746 1.00 36.22 PROT ATOM 222 CA ALA 231 32.497 2.298 21.471 1.00 36.24 PROT ATOM 223 CB ALA 231 31.318 3.255 21.343 1.00 18.90 PROT ATOM 224 C ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 225 O ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 226 N THR 232 34.380 3.434 20.474 1.00 23.74 PROT ATOM 227 CA THR 232 35.329 3.789 19.432 1.00 15.54 PROT ATOM 228 CB THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 229 OG1 THR 232 35.733 5.949 20.460 1.00 16.73 PROT ATOM 230 CG2 THR 232 33.942 5.828 18.891 1.00 2.00 PROT ATOM 231 C THR 232 36.758 3.309 19.670 1.00 19.86 PROT ATOM 232 O THR 232 37.695 3.854 19.094 1.00 15.31 PROT ATOM 234 CA ASN 233 36.938 2.305 20.523 1.00 28.26 PROT ATOM 235 CB ASN 233 38.435 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 38.435 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 39.804 1.689 22.801 1.00 54.02 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 238 ND2 ASN 233 40.045 1.296 24.045 1.00 48.67 PROT ATOM 238 ND2 ASN 233 40.045 1.296 24.045 1.00 48.67 PROT	ATOM	216 CB VAL 230	33.960 1.388 25.528 1.00 33.11	PROT
ATOM 219 C VAL 230 34.224 1.781 23.100 1.00 33.12 PROT ATOM 220 O VAL 230 34.703 0.897 22.385 1.00 40.80 PROT ATOM 221 N ALA 231 33.170 2.507 22.746 1.00 36.22 PROT ATOM 222 CA ALA 231 32.497 2.298 21.471 1.00 36.24 PROT ATOM 223 CB ALA 231 31.318 3.255 21.343 1.00 18.90 PROT ATOM 224 C ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 225 O ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 226 N THR 232 34.380 3.434 20.474 1.00 23.74 PROT ATOM 227 CA THR 232 35.329 3.789 19.432 1.00 15.54 PROT ATOM 228 CB THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 229 OG1 THR 232 35.733 5.949 20.460 1.00 16.73 PROT ATOM 230 CG2 THR 232 33.942 5.828 18.891 1.00 2.00 PROT ATOM 231 C THR 232 36.758 3.309 19.670 1.00 19.86 PROT ATOM 232 O THR 232 37.695 3.854 19.094 1.00 15.31 PROT ATOM 233 N ASN 233 36.938 2.305 20.523 1.00 28.26 PROT ATOM 234 CA ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 235 CB ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 236 CG ASN 233 38.435 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 38.845 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 39.804 1.689 22.801 1.00 54.02 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 238 ND2 ASN 233 40.645 1.296 24.045 1.00 48.67 PROT ATOM 238 ND2 ASN 233 40.045 1.296 24.045 1.00 48.67 PROT	ATOM	217 CG1 VAL 230	34.251 -0.106 25.515 1.00 33.80	PROT
ATOM 220 O VAL 230 34.703 0.897 22.385 1.00 40.80 PROT ATOM 221 N ALA 231 33.170 2.507 22.746 1.00 36.22 PROT ATOM 222 CA ALA 231 32.497 2.298 21.471 1.00 36.24 PROT ATOM 223 CB ALA 231 31.318 3.255 21.343 1.00 18.90 PROT ATOM 224 C ALA 231 33.445 2.501 20.303 1.00 37.54 PROT ATOM 225 O ALA 231 33.342 1.816 19.285 1.00 35.93 PROT ATOM 226 N THR 232 34.380 3.434 20.474 1.00 23.74 PROT ATOM 227 CA THR 232 35.329 3.789 19.432 1.00 15.54 PROT ATOM 228 CB THR 232 35.335 5.321 19.238 1.00 9.70 PROT ATOM 229 OG1 THR 232 35.733 5.949 20.460 1.00 16.73 PROT ATOM 230 CG2 THR 232 33.942 5.828 18.891 1.00 2.00 PROT ATOM 231 C THR 232 36.758 3.309 19.670 1.00 19.86 PROT ATOM 232 O THR 232 37.695 3.854 19.094 1.00 15.31 PROT ATOM 233 N ASN 233 36.938 2.305 20.523 1.00 28.26 PROT ATOM 234 CA ASN 233 38.280 1.771 20.772 1.00 39.32 PROT ATOM 235 CB ASN 233 38.435 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 38.435 1.343 22.234 1.00 47.14 PROT ATOM 236 CG ASN 233 38.804 1.689 22.801 1.00 54.02 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 237 OD1 ASN 233 40.633 2.303 22.128 1.00 60.36 PROT ATOM 238 ND2 ASN 233 40.045 1.296 24.045 1.00 48.67 PROT ATOM 238 ND2 ASN 233 40.045 1.296 24.045 1.00 48.67 PROT	ATOM		34.228 1.985 26.896 1.00 26.54	PROT
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	ATOM	239 C ASN 233	38.507 0.574 19.840 1.00 49.33	PROT

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ATOM		38.338 0.693 18.625 1.00 65.36	PROT
ATOM	241 N ALA 234	38.877 -0.577 20.388 1.00 57.89	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	39.090 -1.752 19.552 1.00 57.22	PROT
ATOM	243 CB ALA 234	40.372 -1.595 18.754 1.00 48.03	PROT
ATOM	244 C ALA 234	39.141 -3.027 20.384 1.00 62.42	PROT
ATOM	245 O- ALA 234	38.471 -3.073 21.440 1.00 56.93	PROT
ATOM	246 OT ALA 234	39.853 -3.968 19.965 1.00 76.16	PROT
ATOM	247 N TRP 239	41.987 -7.449 22.970 1.00 58.82	PROT
ATOM	248 CA TRP 239	43.077 -6.886 22.154 1.00 51.37	PROT
ATOM	249 CB TRP 239	43.325 -5.406 22.534 1.00 45.12	PROT
ATOM	250 CG TRP 239	44.193 -5.170 23.760 1.00 43.09	PROT
ATOM	251 CD2 TRP 239	45.617 -5.037 23.793 1.00 32.36	PROT
ATOM	252 CE2 TRP 239	45.990 -4.872 25.142 1.00 28.37	PROT
ATOM	253 CE3 TRP 239	46.615 -5.049 22.813 1.00 40.79	PROT
ATOM	254 CD1 TRP 239	43.773 -5.073 25.059 1.00 46.63	PROT
ATOM	255 NE1 TRP 239	44.847 -4.896 25.893 1.00 27.08	PROT
ATOM	256 CZ2 TRP 239	47.315 -4.717 25.535 1.00 35.48	PROT
ATOM	257 CZ3 TRP 239	47.936 -4.896 23.204 1.00 40.18	PROT
ATOM	258 CH2 TRP 239	48.273 -4.733 24.554 1.00 49.93	PROT
ATOM	259 C TRP 239	44.422 -7.623 22.063 1.00 49.76	PROT
ATOM	260 O TRP 239	44.944 -7.799 20.962 1.00 48.14	PROT
ATOM ATOM	261 N LYS 240 262 CA LYS 240	44.975 -8.048 23.198 1.00 38.92	PROT
ATOM		46.263 -8.735 23.232 1.00 37.29	PROT
ATOM	263 CB LYS 240 264 CG LYS 240	46.572 -9.196 24.657 1.00 38.79	PROT
ATOM	265 CD LYS 240	47.106 -8.099 25.571 1.00 38.43 48.307 -8.584 26.370 1.00 35.71	PROT
ATOM	266 CE LYS 240		PROT
ATOM	267 NZ LYS 240		PROT
ATOM	268 C LYS 240	49.058 -8.377 28.750 1.00 28.85 46.404 -9.914 22.269 1.00 42.18	PROT
ATOM	269 O LYS 240	47.491 -10.132 21.732 1.00 45.89	PROT
ATOM	270 N GLN 241	45.331 -10.679 22.058 1.00 46.08	PROT PROT
ATOM	271 CA GLN 241	45.390 -11.816 21.133 1.00 45.02	PROT
ATOM	272 CB GLN 241	44.575 -13.011 21.638 1.00 46.30	PROT
ATOM	273 CG GLN 241	44.284 -13.018 23.116 1.00 60.38	PROT
ATOM	274 CD GLN 241	42.828 -13.312 23,408 1.00 63.76	PROT
ATOM	275 OE1 GLN 241	42.154 -13.988 22.631 1.00 66.34	PROT
ATOM	276 NE2 GLN 241	42.333 -12.801 24.531 1.00 69.18	PROT
ATOM	277 C GLN 241	44.866 -11.405 19.764 1.00 45.77	PROT
ATOM	278 O GLN 241	45.107 -12.085 18.765 1.00 51.18	PROT
ATOM	279 N LYS 242	44.132 -10.300 19.723 1.00 42.04	PROT
ATOM	280 CA LYS 242	43.613 -9.794 18.464 1.00 48.33	PROT
ATOM	281 CB LYS 242	42.498 -8.786 18.727 1.00 40.17	PROT
ATOM	282 C LYS 242	44.796 -9.123 17.742 1.00 53.04	PROT
ATOM	283 O LYS 242	44.709 -8.753 16.565 1.00 48.21	PROT
ATOM	284 N ARG 243	45.906 -8.992 18.470 1.00 45.44	PROT
ATOM	285 CA ARG 243	47.128 -8.374 17.965 1.00 43.53	PROT
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ATOM	••	48.108 -8.135 19.118 1.00 40.21	PROT
ATOM	287 C ARG 243	47.795 -9.220 16.892 1.00 45.96	PROT
ATOM	288 O ARG 243	47.684 -10.443 16.894 1.00 50.22	PROT
ATOM	289 N LYS 244	48.498 -8.551 15.982 1.00 52.12	PROT
ATOM	290 CA LYS 244	49.202 -9.202 14.879 1.00 45.30	PROT
ATOM	291 CB LYS 244	48.466 -8.950 13.558 1.00 48.24	PROT
ATOM	292 CG LYS 244	47.109 -9.631 13.446 1.00 53.78	PROT
ATOM	293 CD LYS 244	46.835 -10.078 12.011 1.00 60.50	PROT
ATOM	294 CE LYS 244	46.038 -9.030 11.241 1.00 61.03	PROT
ATOM	295 NZ LYS 244	45.455 -7.997 12.146 1.00 55.25	PROT
ATOM	296 C LYS 244	50.616 -8.641 14.786 1.00 40.33	PROT
ATOM	297 O LYS 244	50.849 -7.629 14.125 1.00 36.07	PROT
ATOM	298 N PHE 245	51.556 -9.312 15.445 1.00 27.87	PROT
ATOM	299 CA PHE 245	52.949 -8.885 15.461 1.00 30.61	PROT
ATOM	300 CB PHE 245	53.784 -9.887 16.253 1.00 20.28	PROT
ATOM	301 CG PHE 245	53.454 -9.922 17.713 1.00 37.23	PROT
ATOM	302 CD1 PHE 245	52.636 -10.917 18.234 1.00 40.93	PROT
ATOM	303 CD2 PHE 245	53.958 -8.959 18.577 1.00 41.60	PROT
ATOM	304 CE1 PHE 245	52.326 -10.953 19.594 1.00 42.54	PROT
ATOM	305 CE2 PHE 245	53.652 -8.989 19.936 1.00 45.84	PROT
ATOM	306 CZ PHE 245	52.835 -9.988 20.443 1.00 33.72	PROT
ATOM	307 C PHE 245	53.549 -8.693 14.068 1.00 38.75	PROT
ATOM	308 O PHE 245	53.794 -9.660 13.337 1.00 48.93	PROT
ATOM	309 N LEU 246	53.789 -7.437 13.704 1.00 41.18	PROT
ATOM	310 CA LEU 246	54.362 -7.124 12.404 1.00 43.43	PROT
ATOM	311 CB LEU 246	54.378 -5.612 12.181 1.00 42.78	PROT
ATOM	312 CG LEU 246	54.535 -5.200 10.718 1.00 49.88	PROT
ATOM	313 CD1 LEU 246	53.528 -4.113 10.365 1.00 40.64	PROT
ATOM	314 CD2 LEU 246	55.966 -4.730 10.485 1.00 48.66	PROT
ATOM	315 C LEU 246	55.777 -7.692 12.250 1.00 42.60	PROT
ATOM	316 O LEU 246	56.677 -7.383 13.028 1.00 45.75	PROT
ATOM	317 N PRO 247	55.977 -8.540 11.233 1.00 50.03	PROT
ATOM	318 CD PRO 247	54.914 -8.924 10.286 1.00 60.17	PROT
ATOM	319 CA PRO 247	57.237 -9.199 10.894 1.00 49.90	PROT
ATOM	320 CB PRO 247	57.181 -9.282 9.369 1.00 59.51	PROT
ATOM	321 CG PRO 247	55.678 -9.244 9.023 1.00 52.86	PROT
ATOM	322 C PRO 247	58.499 -8.494 11.392 1.00 48.85	PROT
ATOM	323 O PRO 247	58.675 -7.295 11.186 1.00 49.28	PROT
ATOM	324 N GLU 248	59.379 -9.261 12.032 1.00 47.62	PROT
ATOM	325 CA GLU 248	60.628 -8.733 12.574 1.00 51.41	PROT
ATOM	326 CB GLU 248	61.266 -9.750 13.522 1.00 44.22	PROT
ATOM	327 C GLU 248	61.623 -8.354 11.490 1.00 53.28	PROT
ATOM	328 O GLU 248	62.815 -8.214 11.765 1.00 62.57	PROT
ATOM	329 N ASP 249	61.146 -8.200 10.258 1.00 56.20	PROT
ATOM	330 CA ASP 249	62.030 -7.818 9.164 1.00 55.88	PROT
ATOM	331 CB ASP 249	62.231 -8.981 8.173 1.00 53.88	PROT

ATOM	332 CG ASP 249	60.928 -9.637 7.739 1.00 54.39	PROT
ATOM	333 OD1 ASP 249	60.578 -10.693 8.310 1.00 57.70	PROT
ATOM	334 OD2 ASP 249	60.264 -9.112 6.819 1.00 45.76	PROT
ATOM	335 C ASP 249	61.539 -6.567 8.437 1.00 54.20	PROT
ATOM	336 O ASP 249	62.119 -6.154 7.429 1.00 55.31	PROT
ATOM	337 N. ILE 250	60.469 -5.965 8.954 1.00 46.13	PROT
ATOM	338 CA ILE 250	59.933 -4.735 8.376 1.00 46.12	PROT
ATOM	339 CB ILE 250	58.413 -4.764 8.253 1.00 43.38	PROT
ATOM	340 CG2 ILE 250	57.892 -3.344 8.057 1.00 39.15	PROT
ATOM	341 CG1 ILE 250	58.007 -5.654 7.074 1.00 48.96	PROT
ATOM	342 CD1 ILE 250	56.707 -6.401 7.283 1.00 43.14	PROT
ATOM	343 C ILE 250	60.311 -3.590 9.294 1.00 45.32	PROT
ATOM	344 O ILE 250	60.257 -3.724 10.513 1.00 43.74	PROT
ATOM	345 N GLY 251	60.680 -2.459 8.711 1.00 36.80	PROT
ATOM	346 CA GLY 251	61.091 -1.329 9.521 1.00 39.28	PROT
ATOM	347 C GLY 251	62.370 -1.621 10.305 1.00 44.31	PROT
ATOM	348 O GLY 251	62.538 -1.145 11.428 1.00 51.39	PROT
ATOM	349 N GLN 252	63.277 -2.399 9.715 1.00 55.47	PROT
ATOM	350 CA GLN 252	64.536 -2.745 10.374 1.00 54.24	PROT
ATOM	351 CB GLN 252	64.792 -4.237 10.245 1.00 49.31	PROT
ATOM	352 C GLN 252	65.720 -1.959 9.812 1.00 54.86	PROT
ATOM	353 O GLN 252	65.492 -1.079 8.953 1.00 58.80	PROT
ATOM	354 CB VAL 264	60.887 6.759 5.510 1.00 34.33	PROT
ATOM	355 CG1 VAL 264	59.550 6.086 5.790 1.00 34.34	PROT
ATOM	356 CG2 VAL 264	60.893 8.163 6.080 1.00 20.22	PROT
ATOM	357 C VAL 264	62.053 4.557 5.439 1.00 34.08	PROT
ATOM	358 O VAL 264	62.280 4.466 4.232 1.00 46.39	PROT
ATOM	359 N VAL 264	63.361 6.605 5.966 1.00 21.27	PROT
ATOM	360 CA VAL 264	62.041 5.920 6.122 1.00 29.68	PROT
ATOM	.361 N ASP 265	61.809 3.499 6.209 1.00 40.63	PROT
ATOM	362 CA ASP 265	61.796 2.141 5.670 1.00 43.58	PROT
ATOM	363 CB ASP 265	61.243 1.160 6.704 1.00 44.07	PROT
ATOM	364 CG ASP 265	61.179 -0.262 6.185 1.00 49.19	PROT
ATOM	365 OD1 ASP 265	62.223 -0.945 6.175 1.00 57.67	PROT
ATOM	366 OD2 ASP 265	60.082 -0.702 5.789 1.00 54.75	PROT
ATOM	367 C ASP 265	60.956 2.071 4.401 1.00 48.03	PROT
ATOM	368 O ASP 265	61.362 1.458 3.411 1.00 57.44	PROT
ATOM	369 N LEU 266 370 CA LEU 266	59.793 2.711 4.436 1.00 40.55	PROT
ATOM		58.879 2.741 3.295 1.00 45.78	PROT
ATOM ATOM	371 CB LEU 266 372 CG LEU 266	59.638 2.962 1.977 1.00 45.92	PROT
		59.881 4.407 1.506 1.00 48.41	PROT
ATOM	373 CD1 LEU 266	59.934 4.432 -0.007 1.00 32.83	PROT
ATOM	374 CD2 LEU 266	58.787 5.344 2.012 1.00 45.08 58.064 1.462 2.214 1.00 45.45	PROT
ATOM	375 C LEU 266	58.064 1.462 3.214 1.00 45.45	PROT
ATOM	376 O LEU 266	56.862 1.503 2.949 1.00 42.92	PROT
ATOM	377 N GLU 267	58.712 0.324 3.431 1.00 46.47	PROT

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ATOM	378 CA GLU 267	57.986 -0.935 3.415 1.00 44.34	PROT
ATOM	379 CB GLU 267		PROT
ATOM	380 CG GLU 267		PROT
ATOM	381 CD GLU 267		PROT
ATOM	382 OE1 GLU 267	60.103 -4.470 4.361 1.00 68.92	PROT
ATOM	383 OE2 GLU 267		PROT
ATOM	384 C GLU 267	57.106 -0.880 4.655 1.00 41.57	PROT
ATOM	385 O GLU 267	55.991 -1.398 4.673 1.00 48.68	PROT
ATOM	386 N ALA 268	57.620 -0.215 5.686 1.00 39.33	PROT
ATOM	387 CA ALA 268	56.916 -0.057 6.951 1.00 31.62	PROT
ATOM	388 CB ALA 268	57.918 0.134 8.063 1.00 7.56	PROT
ATOM	389 C ALA 268	55.960 1.135 6.888 1.00 25.96	PROT
ATOM	390 O ALA 268	54.786 1.036 7.237 1.00 17.35	PROT
ATOM	391 N PHE 269	56.464 2.274 6.446 1.00 11.34	PROT
ATOM	392 CA PHE 269	55.615 3.453 6.335 1.00 15.72	PROT
ATOM	393 CB PHE 269	56.274 4.474 5.405 1.00 20.08	PROT
ATOM	394 CG PHE 269	55.552 5.788 5.334 1.00 24.67	PROT
ATOM	395 CD1 PHE 269	55.661 6.713 6.369 1.00 15.69	PROT
ATOM	396 CD2 PHE 269	54.772 6.111 4.222 1.00 20.64	PROT
ATOM	397 CE1 PHE 269	55.003 7.942 6.300 1.00 22.55	PROT
ATOM	398 CE2 PHE 269	54.108 7.342 4.143 1.00 19.77	PROT
ATOM	399 CZ PHE 269	54.224 8.257 5.186 1.00 19.27	PROT
ATOM	400 C PHE 269	54.277 3.010 5.754 1.00 19.45	PROT
ATOM	401 O PHE 269	53.212 3.351 6.261 1.00 13.40	PROT
ATOM	402 N SER 270	54.367 2.214 4.692 1.00 43.85	PROT
ATOM	403 CA SER 270	53.217 1.686 3.967 1.00 46.67	PROT
ATOM	404 CB SER 270	53.687 0.669 2.924 1.00 53.60	PROT
ATOM	405 OG SER 270	52.662 0.382 1.988 1.00 68.82	PROT
ATOM	406 C SER 270	52.181 1.039 4.865 1.00 43.32	PROT
ATOM	407 O SER 270	51.024 1.459 4.893 1.00 43.87	PROT
ATOM	408 N HIS 271	52.594 0.009 5.590 1.00 34.59	PROT
ATOM	409 CA HIS 271	51.681 -0.694 6.486 1.00 37.12	PROT
ATOM	410 CB HIS 271	52.441 -1.772 7.266 1.00 46.61	PROT
ATOM	411 CG HIS 271	52.603 -3.056 6.512 1.00 63.99	PROT
ATOM	412 CD2 HIS 271	51.879 -4.201 6.533 1.00 62.06	PROT
ATOM	413 ND1 HIS 271	53.608 -3.256 5.590 1.00 60.86	PROT
ATOM	414 CE1 HIS 271	53.497 -4.467 5.075 1.00 60.70	PROT
ATOM	415 NE2 HIS 271	52.456 -5.061 5.630 1.00 64.10	PROT
ATOM	416 C HIS 271	50.973 0.261 7.459 1.00 36.53	PROT
ATOM	417 O HIS 271	49.744 0.245 7.586 1.00 37.75	PROT
ATOM	418 N PHE 272	51.752 1.099 8.133 1.00 32.81	PROT
ATOM	419 CA PHE 272	51.190 2.038 9.085 1.00 27.77	PROT
ATOM	420 CB PHE 272	52.302 2.886 9.714 1.00 10.49	PROT
ATOM	421 CG PHE 272	53.338 2.086 10.459 1.00 6.98	PROT
ATOM	422 CD1 PHE 272	54.671 2.478 10.449 1.00 4.13	PROT
ATOM	423 CD2 PHE 272	52.978 0.961 11.193 1.00 6.95	PROT

ATOM	424 CE1 PHE 272	55.634 1.764 11.163 1.00 7.86	PROT
ATOM	425 CE2 PHE 272	53.930 0.242 11.909 1.00 6.13	PROT
ATOM	426 CZ PHE 272	55.263 0.645 11.895 1.00 8.93	PROT
ATOM	427 C PHE 272	50.168 2.939 8.405 1.00 30.96	PROT
ATOM	428 O PHE 272	49.071 3.156 8.931 1.00 30.21	PROT
ATOM	429 N. THR 273	50.522 3.452 7.231 1.00 31.55	PROT
ATOM	430 CA THR 273	49.633 4.343 6.487 1.00 33.39	PROT
ATOM	431 CB THR 273	50.335 4.912 5.243 1.00 36.80	PROT
ATOM	432 OG1 THR 273	50.649 3.847 4.332 1.00 27.42	PROT
ATOM	433 CG2 THR 273	51.613 5.641 5.656 1.00 32.25	PROT
ATOM	434 C THR 273	48.350 3.647 6.056 1.00 34.07	PROT
ATOM	435 O THR 273	47.362 4.294 5.697 1.00 17.11	PROT
ATOM	436 N LYS 274	48.372 2.321 6.088 1.00 34.47	PROT
ATOM	437 CA LYS 274	47.196 1.555 5.726 1.00 42.17	PROT
ATOM	438 CB LYS 274	47.544 0.069 5.615 1.00 40.02	PROT
ATOM.	439 C LYS 274	46.153 1.778 6.818 1.00 41.47	PROT
ATOM	440 O LYS 274	45.115 2.402 6.584 1.00 47.37	PROT
ATOM	441 N ILE 275	46.456 1.290 8.019 1.00 34.08	PROT
ATOM	442 CA ILE 275	45.559 1.403 9.166 1.00 25.49	PROT
ATOM	443 CB ILE 275	45.991 0.435 10.262 1.00 19.72	PROT
ATOM	444 CG2 ILE 275	46.290 -0.934 9.642 1.00 23.39	PROT
ATOM	445 CG1 ILE 275	47.249 0.958 10.953 1.00 12.96	PROT
ATOM	446 CD1 ILE 275	47.970 -0.103 11.769 1.00 11.07	PROT
ATOM	447 C ILE 275	45.440 2.805 9.762 1.00 20.03	PROT
ATOM	448 O ILE 275	44.541 3.081 10.547 1.00 18.98	PROT
ATOM	449 N ILE 276	46.347 3.694 9.402 1.00 8.88	PROT
ATOM ATOM	450 CA ILE 276 451 CB ILE 276	46.268 5.043 9.924 1.00 6.62	PROT
ATOM	451 CB ILE 276 452 CG2 ILE 276	47.298 5.972 9.261 1.00 21.77	PROT
ATOM	452 CG2 ILE 276 453 CG1 ILE 276	46.894 6.267 7.831 1.00 27.28 47.374 7.288 10.028 1.00 6.75	PROT
ATOM	454 CD1 ILE 276	48.349 7.255 11.153 1.00 15.44	PROT
ATOM	455 C ILE 276	44.887 5.649 9.697 1.00 12.17	PROT PROT
ATOM	456 O ILE 276	44.349 6.331 10.565 1.00 29.36	PROT
ATOM	457 N THR 277	44.303 5.411 8.535 1.00 22.12	PROT
ATOM	458 CA THR 277	43.007 6.005 8.260 1.00 27.16	PROT
ATOM	459 CB THR 277	42.532 5.675 6.834 1.00 27.11	PROT
ATOM	460 OG1 THR 277	43.665 5.584 5.955 1.00 22.55	PROT
ATOM	461 CG2 THR 277	41.594 6.763 6.337 1.00 26.98	PROT
ATOM	462 C THR 277	41.944 5.591 9.270 1.00 25.23	PROT
ATOM	463 O THR 277	41.271 6.443 9.847 1.00 21.62	PROT
ATOM	464 N PRO 278	41.769 4.279 9.491 1.00 18.64	PROT
ATOM	465 CD PRO 278	42.472 3.167 8.832 1.00 9.52	PROT
ATOM	466 CA PRO 278	40.765 3.803 10.453 1.00 18.48	PROT
ATOM	467 CB PRO 278	40.907 2.280 10.415 1.00 14.77	PROT
ATOM	468 CG PRO 278	42.195 2.008 9.738 1.00 7.70	PROT
ATOM	469 C PRO 278	40.956 4.356 11.870 1.00 25.40	PROT
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ATOM	470 O PRO 278	39.983 4.628 12.576 1.00 22.33	PROT
ATOM	471 N ALA 279	42.211 4.507 12.285 1.00 22.14	PROT
ATOM	472 CA ALA 279	42.519 5.038 13.607 1.00 20.26	PROT
ATOM	473 CB ALA 279	44.016 5.033 13.831 1.00 13.33	PROT
ATOM	474 C ALA 279	41.984 6.456 13.699 1.00 16.49	PROT
ATOM	475 O. ALA 279	41.222 6.797 14.598 1.00 32.38	PROT
ATOM	476 N ILE 280	42.384 7.286 12.753 1.00 7.56	PROT
ATOM	477 CA ILE 280	41.935 8.666 12.734 1.00 9.96	PROT
ATOM	478 CB ILE 280	42.422 9.380 11.462 1.00 8.46	PROT
ATOM	479 CG2 ILE 280	42.172 10.871 11.581 1.00 2.00	PROT
ATOM	480 CG1 ILE 280	43.901 9.059 11.220 1.00 10.96	PROT
ATOM	481 CD1 ILE 280	44.615 10.036 10.294 1.00 8.54	PROT
ATOM	482 C ILE 280	40.410 8.805 12.805 1.00 15.46	PROT
ATOM	483 O ILE 280	39.887 9.741 13.421 1.00 24.39	PROT
ATOM	484 N THR 281	39.692 7.883 12.172 1.00 24.18	PROT
ATOM	485 CA THR 281	38.238 7.962 12.153 1.00 24.77	PROT
ATOM	486 CB THR 281	37.650 6.952 11.145 1.00 33.90	PROT
ATOM	487 OG1 THR 281	38.607 6.711 10.108 1.00 34.62	PROT
ATOM	488 CG2 THR 281	36.379 7.506 10.513 1.00 39.80	PROT
ATOM	489 C THR 281	37.655 7.726 13.535 1.00 23.39	PROT
ATOM	490 O THR 281	36.733 8.422 13.960 1.00 19.51	PROT
ATOM	491 N ARG 282	38.213 6.743 14.234 1.00 16.90	PROT
ATOM	492 CA ARG 282	37.781 6.404 15.583 1.00 12.29	PROT
ATOM	493 CB ARG 282	38.641 5.260 16.115 1.00 5.36	PROT
ATOM	494 CG ARG 282	37.936 3.926 16.136 1.00 17.05	PROT
ATOM	495 CD ARG 282	38.296 3.095 14.942 1.00 18.41	PROT
ATOM	496 NE ARG 282	39.622 2.475 15.011 1.00 35.77	PROT
ATOM	497 CZ ARG 282	40.454 2.501 16.055 1.00 36.80	PROT
ATOM	498 NH1 ARG 282	41.629 1.888 15.967 1.00 35.96	PROT
ATOM	499 NH2 ARG 282	40.134 3.120 17.183 1.00 25.20	PROT
ATOM	500 C ARG 282	37.863 7.626 16.520 1.00 16.75	PROT
ATOM	501 O ARG 282	37.078 7.758 17.456 1.00 22.98	PROT
ATOM	502 N VAL 283	38.813 8.518 16.268 1.00 11.92	PROT
ATOM	503 CA VAL 283	38.937 9.719 17.083 1.00 14.68	PROT
ATOM ATOM	504 CB VAL 283 505 CG1 VAL 283	40.191 10.541 16.696 1.00 23.35	PROT
ATOM		40.467 11.593 17.752 1.00 11.98	PROT
ATOM	506 CG2 VAL 283 507 C VAL 283	41.396 9.621 16.526 1.00 20.41	PROT
		37.705 10.580 16.833 1.00 12.72	PROT
ATOM	508 O VAL 283	36.965 10.929 17.752 1.00 20.37	PROT
ATOM ATOM	509 N VAL 284 510 CA VAL 284	37.503 10.920 15.567 1.00 18.28 36.360 11.737 15.150 1.00 16.08	PROT
ATOM		36.369 11.727 15.150 1.00 16.98 36.351 11.765 13.602 1.00 27.40	PROT
		36.251 11.765 13.602 1.00 27.40	PROT
ATOM	512 CG1 VAL 284	35.434 12.973 13.172 1.00 19.30	PROT
ATOM	513 CG2 VAL 284	37.649 11.794 12.959 1.00 16.94 35.112 11.003 15.715 1.00 14.00	PROT
ATOM	514 C VAL 284	35.113 11.093 15.715 1.00 14.89	PROT
ATOM	515 O VAL 284	34.233 11.781 16.219 1.00 10.93	PROT

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ATOM	•	35.046 9.768 15.623 1.00 10.68	PROT
ATOM		33.898 9.022 16.114 1.00 20.76	PROT
ATOM		34.079 7.518 15.874 1.00 22.99	PROT
ATOM		33.985 7.130 14.397 1.00 30.01	PROT
ATOM		33.185 7.735 13.648 1.00 18.56	PROT
ATOM	_ -	34.720 6.202 13,993 1.00 27.74	PROT
ATOM		33.734 9.274 17.604 1.00 26.87	PROT
ATOM	523 O ASP 285	32.609 9.349 18.103 1.00 39.89	PROT
ATOM	524 N PHE 286	34.861 9.405 18.308 1.00 25.45	PROT
ATOM	525 CA PHE 286	34.862 9.654 19.746 1.00 15.66	PROT
ATOM	526 CB PHE 286	36.284 9.533 20.305 1.00 7.30	PROT
ATOM	527 CG PHE 286	36.454 10.104 21.703 1.00 17.92	PROT
ATOM	528 CD1 PHE 286	35.848 9.499 22.805 1.00 19.35	PROT
ATOM	529 CD2 PHE 286	37.229 11.245 21.920 1.00 19.24	PROT
ATOM	530 CE1 PHE 286	36.014 10.021 24.087 1.00 9.94	PROT
ATOM	531 CE2 PHE 286	37.395 11.769 23.207 1.00 11.33	PROT
ATOM	532 CZ PHE 286	36.786 11.154 24.283 1.00 2.00	PROT
ATOM	533 C PHE 286	34.313 11.043 20.030 1.00 17.67	PROT
ATOM	534 O PHE 286	33.367 11.201 20.797 1.00 14.36	PROT
ATOM	535 N ALA 287	34.905 12.056 19.410 1.00 12.57	PROT
ATOM	536 CA ALA 287	34.443 13.426 19.622 1.00 12.49	PROT
ATOM	537 CB ALA 287	35.250 14.386 18.759 1.00 23.54	PROT
ATOM	538 C ALA 287	32.954 13.559 19.307 1.00 9.21	PROT
ATOM	539 O ALA 287	32.209 14.205 20.043 1.00 11.68	PROT
ATOM	540 N LYS 288	32.540 12.929 18.209 1.00 16.43	PROT
ATOM	541 CA LYS 288	31.157 12.944 17.736 1.00 16.10	PROT
ATOM	542 CB LYS 288	31.003 11.977 16.569 1.00 13.15	PROT
ATOM	543 CG LYS 288	31.117 12.636 15.219 1.00 25.55	PROT
ATOM	544 CD LYS 288	30.480 11.779 14.136 1.00 32.95	PROT
ATOM ATOM	545 CE LYS 288 546 NZ LYS 288	31.279 10.507 13.900 1.00 34.58	PROT
ATOM	546 NZ LYS 288 547 C LYS 288	30.755 9.721 12.748 1.00 36.93	PROT
ATOM	548 O LYS 288	30.154 12.569 18.813 1.00 18.87	PROT
ATOM	549 N LYS 289	29.078 13.171 18.917 1.00 12.83	PROT
ATOM	550 CA LYS 289	30.525 11.574 19.614 1.00 11.81 29.674 11.067 20.681 1.00 15.53	PROT
ATOM	550 CA L13 289 551 CB LYS 289		PROT
ATOM	551 CB LTS 289 552 CG LYS 289		PROT
ATOM	552 CO LYS 289		PROT
ATOM	554 CE LYS 289	29.140 7.382 20.471 1.00 28.97 29.951 6.167 20.071 1.00 25.06	PROT
ATOM	555 NZ LYS 289	30.043 6.060 18.590 1.00 39.19	PROT
ATOM	556 C LYS 289	29.660 11.884 21.969 1.00 15.95	PROT
ATOM	557 O LYS 289	29.205 11.398 23.001 1.00 28.53	PROT
ATOM	558 N LEU 290	30.151 13.116 21.919 1.00 10.13	PROT
ATOM	559 CA LEU 290	30.155 13.959 23.104 1.00 7.83	PROT
ATOM	560 CB LEU 290	31.588 14.300 23.532 1.00 14.46	PROT
ATOM	561 CG LEU 290	32.676 13.228 23.542 1.00 14.46	PROT
	201 CG LLU 290	32.010 13.220 23.342 1.00 11.22	PROT

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ATOM		34.016 13.900 23.678 1.00 3.02	PROT
ATOM	563 CD2 LEU 290	32.449 12.257 24.686 1.00 9.39	PROT
ATOM	564 C LEU 290	29.410 15.259 22.849 1.00 7.59	PROT
ATOM	565 O LEU 290	29.942 16.148 22.196 1.00 11.01	PROT
ATOM	566 N PRO 291	28.169 15.381 23.365 1.00 14.33	PROT
ATOM	567 CD PRO 291	27.515 14.291 24.109 1.00 18.52	PROT
ATOM	568 CA PRO 291	27.290 16.556 23.240 1.00 6.61	PROT
ATOM	569 CB PRO 291	26.296 16.400 24.384 1.00 11.95	PROT
ATOM	570 CG PRO 291	26.496 15.004 24.929 1.00 20.22	PROT
ATOM	571 C PRO 291	28.029 17.885 23.332 1.00 14.74	PROT
ATOM	572 O PRO 291	27.795 18.792 22.537 1.00 26.09	PROT
ATOM	573 N MET 292	28.917 18.002 24.315 1.00 24.06	PROT
ATOM	574 CA MET 292	29.697 19.225 24.494 1.00 25.33	PROT
ATOM	575 CB MET 292	30.706 19.046 25.628 1.00 26.65	PROT
ATOM	576 CG MET 292	30.222 19.581 26.962 1.00 26.97	PROT
ATOM	577 SD MET 292	31.153 18.943 28.362 1.00 29.01	PROT
ATOM	578 CE MET 292	30.315 17.438 28.685 1.00 17.91	PROT
ATOM	579 C MET 292	30.430 19.588 23.204 1.00 23.01	PROT
ATOM	580 O MET 292	30.478 20.747 22.813 1.00 31.98	PROT
ATOM	581 N PHE 293	31.007 18.591 22.547 1.00 23.44	PROT
ATOM	582 CA PHE 293	31.724 18.819 21.297 1.00 24.83	PROT
ATOM	583 CB PHE 293	32.389 17.529 20.830 1.00 15.05	PROT
ATOM	584 CG PHE 293	33.214 17.686 19.594 1.00 13.55	PROT
ATOM	585 CD1 PHE 293	34.376 18.446 19.614 1.00 19.86	PROT
ATOM	586 CD2 PHE 293	32.867 17.024 18.425 1.00 22.99	PROT
ATOM	587 CE1 PHE 293	35.184 18.540 18.495 1.00 18.15	PROT
ATOM	588 CE2 PHE 293	33.671 17.108 17.291 1.00 20.83	PROT
ATOM	589 CZ PHE 293	34.831 17.866 17.328 1.00 22.53	PROT
ATOM	590 C PHE 293	30.759 19.291 20.222 1.00 27.26	PROT
ATOM	591 O PHE 293	30.971 20.319 19.577 1.00 28.69	PROT
ATOM	592 N CYS 294	29.689 18.528 20.040 1.00 29.92	PROT
ATOM	593 CA CYS 294	28.700 18.855 19.037 1.00 35.54	PROT
ATOM	594 CB CYS 294	27.540 17.860 19.106 1.00 19.11	PROT
ATOM	595 SG CYS 294	27.843 16.358 18.132 1.00 35.66	PROT
ATOM	596 C CYS 294	28.203 20.291 19.171 1.00 38.84	PROT
ATOM	597 O CYS 294	28.072 20.995 18.169 1.00 45.94	PROT
ATOM	598 N GLU 295	27.959 20.739 20.401 1.00 27.34	PROT
ATOM	599 CA GLU 295	27.472 22.097 20.632 1.00 21.06	PROT
ATOM	600 CB GLU 295	27.178 22.306 22.121 1.00 29.78	PROT
ATOM	601 C GLU 295	28.458 23.158 20.128 1.00 23.67	PROT
ATOM	602 O GLU 295	28.228 24.357 20.272 1.00 29.89	PROT
ATOM	603 N LEU 296	29.551 22.715 19.522 1.00 21.46	PROT
ATOM	604 CA LEU 296	30.545 23.642 19.005 1.00 26.35	PROT
ATOM	605 CB LEU 296 606 CG LEU 296	31.947 23.128 19.330 1.00 25.17	PROT
ATOM		32.419 23.157 20.778 1.00 13.78	PROT
ATOM	607 CD1 LEU 296	33.593 22.217 20.931 1.00 23.61	PROT

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ATOM	.608 CD2 LEU 296	32.814 24.564 21.160 1.00 13.82	PROT
ATOM	609 C LEU 296	30.415 23.783 17.493 1.00 31.88	PROT
ATOM	610 O LEU 296	29.890 22.890 16.827 1.00 45.99	PROT
ATOM	611 N PRO 297	30.884 24.912 16.932 1.00 27.00	PROT
ATOM	612 CD PRO 297	31.423 26.037 17.708 1.00 36.12	PROT
ATOM	613 CA PRO 297	30.856 25.222 15.492 1.00 22.30	PROT
ATOM	614 CB PRO 297	31.182 26.716 15.424 1.00 16.06	PROT
ATOM	615 CG PRO 297	31.107 27.208 16.827 1.00 42.41	PROT
ATOM	616 C PRO 297	31.838 24.413 14.642 1.00 28.19	PROT
ATOM	617 O PRO 297	32.983 24.189 15.036 1.00 39.38	PROT
ATOM	618 N CYS 298	31.371 24.014 13.457 1.00 35.37	PROT
ATOM	619 CA CYS 298	32.134 23.233 12.481 1.00 32.41	PROT
ATOM	620 CB CYS 298	31.416 23.289 11.112 1.00 40.85	PROT
ATOM	621 SG CYS 298	32.431 23.615 9.614 1.00 61.24	PROT
ATOM	622 C CYS 298	33.596 23.654 12.352 1.00 31.68	PROT
ATOM	623 O CYS 298	34.474 22.804 12.225 1.00 28.49	PROT
ATOM	624 N GLU 299	33.869 24.954 12.393 1.00 29.93	PROT
ATOM	625 CA GLU 299	35.253 25.407 12.278 1.00 36.38	PROT
ATOM	626 CB GLU 299	35.346 26.931 12.203 1.00 32.78	PROT
ATOM	627 CG GLU 299	34.467 27.546 11.167 1.00 43.40	PROT
ATOM	628 CD GLU 299	33.038 27.593 11.625 1.00 58.19	PROT
ATOM	629 OE1 GLU 299	32.723 28.457 12.474 1.00 67.37	PROT
ATOM	630 OE2 GLU 299	32.237 26.762 11.143 1.00 54.02	PROT
ATOM	631 C GLU 299	36.057 24.932 13.475 1.00 38.89	PROT
ATOM	632 O GLU 299	37.129 24.342 13.316 1.00 48.67	PROT
ATOM	633 N ASP 300	35.528 25.186 14.671 1.00 36.49	PROT
ATOM	634 CA ASP 300	36.201 24.805 15.906 1.00 29.96	PROT
ATOM	635 CB ASP 300	35.455 25.391 17.111 1.00 5.33	PROT
ATOM	636 CG ASP 300	35.830 26.853 17.378 1.00 19.10	PROT
ATOM	637 OD1 ASP 300	36.491 27.473 16.518 1.00 27.28	PROT
ATOM	638 OD2 ASP 300	35.470 27.396 18.444 1.00 23.55	PROT
ATOM	639 C ASP 300	36.380 23.294 16.054 1.00 25.88	PROT
ATOM	640 O ASP 300	37.441 22.845 16.484 1.00 19.03	PROT
ATOM	641 N GLN 301	35.360 22.516 15.689 1.00 6.29	PROT
ATOM	642 CA GLN 301	35.432 21.055 15.769 1.00 9.51	PROT
ATOM	643 CB GLN 301	34.170 20.421 15.183 1.00 18.27	PROT
ATOM	644 CG GLN 301	32.886 20.813 15.875 1.00 28.72	PROT
ATOM	645 CD GLN 301	31.676 20.155 15.243 1.00 17.63	PROT
ATOM	646 OE1 GLN 301	31.689 19.823 14.060 1.00 30.65	PROT
ATOM	647 NE2 GLN 301	30.625 19.965 16.027 1.00 30.44	PROT
ATOM	648 C GLN 301	36.646 20.491 15.020 1.00 15.48	PROT
ATOM	649 O GLN 301	37.333 19.584 15.500 1.00 21.96	PROT
ATOM	650 N ILE 302	36.891 21.014 13.825 1.00 24.00	PROT
ATOM	651 CA ILE 302	38.011 20.555 13.026 1.00 28.84	PROT
ATOM	652 CB ILE 302	37.930 21.112 11.607 1.00 33.13	PROT
ATOM	653 CG2 ILE 302	39.147 20.690 10.813 1.00 37.90	PROT

ATOM		36.656 20.610 10.941 1.00 29.63	PROT
ATOM	655 CD1 ILE 302	36.296 21.356 9.698 1.00 32.99	PROT
ATOM	656 C ILE 302	39.308 21.014 13.670 1.00 28.73	PROT
ATOM	657 O ILE 302	40.219 20.219 13.895 1.00 36.02	PROT
ATOM	658 N ILE 303	39.396 22.304 13.968 1.00 25.04	PROT
ATOM	659 CA ILE 303	40.590 22.817 14.603 1.00 24.27	PROT
ATOM	660 CB ILE 303	40.414 24.270 15.054 1.00 20.89	PROT
ATOM	661 CG2 ILE 303	41.686 24.740 15.744 1.00 32.38	PROT
ATOM	662 CG1 ILE 303	40.079 25.158 13.849 1.00 18.88	PROT
ATOM	663 CD1 ILE 303	40.298 26.648 14.079 1.00 5.31	PROT
ATOM	664 C ILE 303	40.861 21.948 15.825 1.00 26.92	PROT
ATOM	665 O ILE 303	41.963 21.440 15.997 1.00 31.32	PROT
ATOM	666 N LEU 304	39.843 21.763 16.659 1.00 11.00	PROT
ATOM	667 CA LEU 304	39.983 20.953 17.854 1.00 7.21	PROT
ATOM	668 CB LEU 304	38.663 20.886 18.613 1.00 2.00	PROT
ATOM	669 CG LEU 304	38.633 21.511 20.012 1.00 8.04	PROT
ATOM	670 CD1 LEU 304	39.383 22.812 19.997 1.00 2.00	PROT
ATOM	671 CD2 LEU 304	37.188 21.729 20.472 1.00 4.99	PROT
ATOM	672 C LEU 304	40.441 19.554 17.507 1.00 4.64	PROT
ATOM	673 O LEU 304	41.368 19.032 18.119 1.00 14.88	PROT
ATOM	674 N LEU 305	39.807 18.953 16.510 1.00 4.55	PROT
ATOM	675 CA LEU 305	40.140 17.590 16.093 1.00 7.03	PROT
ATOM	676 CB LEU 305	39.099 17.098 15.104 1.00 3.70	PROT
ATOM	677 CG LEU 305	38.164 16.054 15.691 1.00 10.31	PROT
ATOM	678 CD1 LEU 305	36.744 16.340 15.245 1.00 2.00	PROT
ATOM	679 CD2 LEU 305	38.629 14.665 15.260 1.00 9.42	PROT
ATOM	680 C LEU 305	41.527 17.418 15.483 1.00 10.17	PROT
ATOM	681 O LEU 305	42.174 16.374 15.651 1.00 7.58	PROT
ATOM	682 N LYS 306	41.975 18.442 14.765 1.00 9.98	PROT
ATOM	683 CA LYS 306	43.283 18.408 14.127 1.00 9.14	PROT
ATOM	684 CB LYS 306	43.409 19.558 13.131 1.00 18.85	PROT
ATOM	685 CG LYS 306	42.815 19.270 11.763 1.00 25.44	PROT
ATOM	686 CD LYS 306	42.198 20.529 11.178 1.00 29.07	PROT
ATOM	687 CE LYS 306	42.698 20.808 9.774 1.00 37.81	PROT
ATOM	688 NZ LYS 306	43.867 19.964 9.403 1.00 30.48	PROT
ATOM	689 C LYS 306	44.376 18.522 15.175 1.00 7.31	PROT
ATOM	690 O LYS 306	45.439 17.919 15.048 1.00 16.95	PROT
ATOM	691 N GLY 307	44.097 19.295 16.218 1.00 12.67	PROT
ATOM	692 CA GLY 307	45.062 19.484 17.279 1.00 7.25	PROT
ATOM	693 C GLY 307	45.297 18.269 18.150 1.00 15.08	PROT
ATOM	694 O GLY 307	46.441 17.972 18.488 1.00 20.11	PROT
ATOM	695 N CYS 308	44.225 17.552 18.481 1.00 8.29	PROT
ATOM	696 CA CYS 308	44.286 16.380 19.364 1.00 3.44	PROT
ATOM	697 CB CYS 308	43.097 16.402 20.326 1.00 14.26	PROT
ATOM	698 SG CYS 308	41.539 15.750 19.634 1.00 21.83	PROT
ATOM	699 C CYS 308	44.344 14.995 18.738 1.00 8.37	PROT

ATOM	700 O CYS 308	44.502 13.997 19.453 1.00 10.98	PROT
ATOM	701 N CYS 309	44.202 14.916 17.420 1.00 10.83	PROT
ATOM	702 CA CYS 309	44.236 13.625 16.752 1.00 3.22	PROT
ATOM	703 CB CYS 309	44.240 13.831 15.240 1.00 15.79	PROT
ATOM	704 SG CYS 309	43.683 12.402 14.319 1.00 25.54	PROT
ATOM	705 C- CYS 309	45.439 12.767 17.193 1.00 2.00	PROT
ATOM	706 O CYS 309	45.251 11.722 17.807 1.00 12.28	PROT
ATOM	707 N MET 310	46.663 13.205 16.900 1.00 2.00	PROT
ATOM	708 CA MET 310	47.858 12.446 17.286 1.00 2.00	PROT
ATOM	709 CB MET 310	49.122 13.171 16.860 1.00 2.00	PROT
ATOM	710 CG MET 310	49.975 12.422 15.880 1.00 5.92	PROT
ATOM	711 SD MET 310	50.481 10.805 16.368 1.00 22.47	PROT
ATOM	712 CE MET 310	52.140 11.112 16.808 1.00 20.84	PROT
ATOM	713 C MET 310	47.941 12.239 18.793 1.00 11.95	PROT
ATOM	714 O MET 310	48.455 11.220 19.270 1.00 15.53	PROT
ATOM	715 N GLU 311	47.463 13.225 19.542 1.00 6.79	PROT
ATOM	716 CA GLU 311	47.493 13.139 20.979 1.00 2.00	PROT
ATOM	717 CB GLU 311	46.932 14.427 21.581 1.00 6.42	PROT
ATOM	718 CG GLU 311	47.880 15.619 21.436 1.00 8.40	PROT
ATOM	719 CD GLU 311	47.236 16.940 21.820 1.00 14.10	PROT
ATOM	720 OE1 GLU 311	46.157 16.895 22.434 1.00 16.54	PROT
ATOM	721 OE2 GLU 311	47.795 18.020 21.515 1.00 4.09	PROT
ATOM	722 C GLU 311	46.683 11.923 21.406 1.00 7.80	PROT
ATOM	723 O GLU 311	47.195 11.026 22.067 1.00 14.07	PROT
ATOM	724 N ILE 312	45.425 11.873 21.001 1.00 2.00	PROT
ATOM	725 CA ILE 312	44.574 10.752 21.371 1.00 3.60	PROT
ATOM	726 CB ILE 312	43.114 11.013 20.947 1.00 2.00	PROT
ATOM	727 CG2 ILE 312	42.277 9.769 21.145 1.00 2.00	PROT
ATOM	728 CG1 ILE 312	42.579 12.221 21.727 1.00 2.00	PROT
ATOM ATOM	729 CD1 ILE 312 730 C ILE 312	41.118 12.555 21.495 1.00 2.00	PROT
ATOM	730 C ILE 312 731 O ILE 312	45.049 9.437 20.760 1.00 8.32 44.918 8.373 21.370 1.00 5.58	PROT
ATOM	731 O ILE 312 732 N MET 313	44.918 8.373 21.370 1.00 5.58 45.615 9.501 19.563 1.00 3.98	PROT
ATOM	732 IN MET 313	46.054 8.282 18.905 1.00 8.91	PROT PROT
ATOM	734 CB MET 313	46.455 8.572 17.462 1.00 25.71	PROT
ATOM	735 CG MET 313	45.430 8.111 16.431 1.00 22.86	PROT
ATOM	736 SD MET 313	45.955 8.430 14.736 1.00 20.60	PROT
ATOM	737 CE MET 313	45.412 10.055 14.534 1.00 14.95	PROT
ATOM	738 C MET 313	47.211 7.634 19.635 1.00 12.95	PROT
ATOM	739 O MET 313	47.213 6.426 19.857 1.00 22.09	PROT
ATOM	740 N SER 314	48.190 8.442 20.021 1.00 10.79	PROT
ATOM	741 CA SER 314	49.354 7.935 20.719 1.00 2.00	PROT
ATOM	742 CB SER 314	50.399 9.042 20.816 1.00 7.24	PROT
ATOM	743 OG SER 314	50.453 9.815 19.619 1.00 10.89	PROT
ATOM	744 C SER 314	48.991 7.399 22.105 1.00 8.64	PROT
ATOM	745 O SER 314	49.559 6.392 22.558 1.00 5.72	PROT
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ATOM 746 N LEU 315 48.050 8.062 22.782 1.00 2.00 ATOM 747 CA LEU 315 47.628 7.605 24.104 1.00 2.00 ATOM 748 CB LEU 315 46.521 8.502 24.671 1.00 2.95 ATOM 749 CG LEU 315 45.831 8.096 25.992 1.00 2.00 ATOM 750 CD1 LEU 315 46.876 7.845 27.072 1.00 2.54	PROT PROT PROT PROT PROT PROT
ATOM 748 CB LEU 315 46.521 8.502 24.671 1.00 2.95 ATOM 749 CG LEU 315 45.831 8.096 25.992 1.00 2.00	PROT PROT PROT PROT
ATOM 749 CG LEU 315 45.831 8.096 25.992 1.00 2.00	PROT PROT PROT
100 2.00	PROT PROT
ATOM 750 CD1 LEU 315 46.876 7.845 27.072 1.00 2.54	PROT
100 2.54	
ATOM 751 CD2 LEU 315 44.865 9.182 26.444 1.00 2.00	
ATOM 752 C LEU 315 47.107 6.182 23.945 1.00 3.25	PROT
ATOM 753 O LEU 315 47.568 5.253 24.603 1.00 2.00	PROT
ATOM 754 N ARG 316 46.157 6.010 23.039 1.00 7.28	PROT
ATOM 755 CA ARG 316 45.588 4.691 22.808 1.00 13.31	PROT
ATOM 756 CB ARG 316 44.551 4.758 21.693 1.00 11.11	PROT
ATOM 757 CG ARG 316 43.545 5.872 21.887 1.00 10.55	PROT
ATOM 758 CD ARG 316 42.354 5.639 21.012 1.00 10.09	PROT
ATOM 759 NE ARG 316 41.131 6.149 21.605 1.00 12.29	PROT
ATOM 760 CZ ARG 316 39.955 6.127 20.994 1.00 6.99	PROT
ATOM 761 NH1 ARG 316 38.880 6.608 21.595 1.00 19.32	PROT
ATOM 762 NH2 ARG 316 39.853 5.619 19.778 1.00 17.16	PROT
ATOM 763 C ARG 316 46.666 3.686 22.458 1.00 10.10	PROT
ATOM 764 O ARG 316 46.549 2.508 22.753 1.00 14.94	PROT
ATOM 765 N ALA 317 47.723 4.148 21.819 1.00 6.51	PROT
ATOM 766 CA ALA 317 48.801 3.243 21.474 1.00 11.04	PROT
ATOM 767 CB ALA 317 49.749 3.902 20.487 1.00 16.13	PROT
ATOM 768 C ALA 317 49.539 2.910 22.753 1.00 12.70	PROT
ATOM 769 O ALA 317 49.822 1.755 23.033 1.00 23.09	PROT
ATOM 770 N ALA 318 49.832 3.943 23.534 1.00 14.79	PROT
ATOM 771 CA ALA 318 50.567 3.779 24.776 1.00 8.38	PROT
ATOM 772 CB ALA 318 50.727 5.122 25.448 1.00 11.75	PROT
	PROT
	PROT
	PROT
ATOM 776 CA VAL 319 48.002 2.131 27.027 1.00 9.64	PROT
ATOM 777 CB VAL 319 46.579 2.622 27.334 1.00 2.57	PROT
ATOM 778 CG1 VAL 319 46.644 3.929 28.127 1.00 5.09	PROT
ATOM 779 CG2 VAL 319 45.807 2.823 26.043 1.00 5.15	PROT
	PROT
	PROT
	PROT
ATOM 783 CA ARG 320 48.405 -0.902 24.767 1.00 13.20	PROT
	PROT
ATOM 785 CG ARG 320 46.310 -0.405 23.420 1.00 14.07	PROT
ATOM 786 CD ARG 320 45.283 -1.460 23.035 1.00 19.69	PROT
ATOM 787 NE ARG 320 44.168 -0.868 22.292 1.00 36.52	PROT
	PROT
ATOM 789 NH1 ARG 320 41.966 -0.705 21.609 1.00 43.57	PROT
ATOM 790 NH2 ARG 320 42.596 -2.367 23.061 1.00 49.93	PROT
ATOM 791 C ARG 320 49.835 -1.391 24.662 1.00 15.45 1	PROT

ATOM	792 O ARG 320	50.167 -2.218 23.809 1.00 24.78	PROT
ATOM	793 N TYR 321	50.684 -0.860 25.537 1.00 13.68	PROT
ATOM	794 CA TYR 321	52.085 -1.258 25.572 1.00 18.80	PROT
ATOM	795 CB TYR 321	52.925 -0.208 26.295 1.00 9.64	PROT
ATOM	796 CG TYR 321	54.313 -0.685 26.622 1.00 11.20	PROT
ATOM	797 CD1 TYR 321	55.211 -1.005 25.612 1.00 2.00	PROT
ATOM	798 CE1 TYR 321	56.483 -1.461 25.906 1.00 9.63	PROT
ATOM	799 CD2 TYR 321	54.727 -0.834 27.943 1.00 18.93	PROT
ATOM	800 CE2 TYR 321	56.003 -1.293 28.250 1.00 19.49	PROT
ATOM	801 CZ TYR 321	56.874 -1.604 27.225 1.00 14.75	PROT
ATOM	802 OH TYR 321	58.137 -2.053 27.518 1.00 22.96	PROT
ATOM	803 C TYR 321	52.209 -2.607 26.287 1.00 19.74	PROT
ATOM	804 O TYR 321	51.483 -2.889 27.242 1.00 31.56	PROT
ATOM	805 N ASP 322	53.136 -3.435 25.823 1.00 26.35	PROT
ATOM	806 CA ASP 322	53.346 -4.759 26.392 1.00 22.38	PROT
ATOM	807 CB ASP 322	52.982 -5.814 25.353 1.00 33.63	PROT
ATOM	808 CG ASP 322	52.601 -7.128 25.970 1.00 40.70	PROT
ATOM	809 OD1 ASP 322	51.539 -7.658 25.591 1.00 48.18	PROT
ATOM	810 OD2 ASP 322	53.358 -7.628 26.826 1.00 38.91	PROT
ATOM	811 C ASP 322	54.800 -4.928 26.776 1.00 23.51	PROT
ATOM	812 O ASP 322	55.683 -4.844 25.924 1.00 37.80	PROT
ATOM	813 N PRO 323	55.076 -5.160 28.066 1.00 24.06	PROT
ATOM	814 CD PRO 323	54.130 -5.258 29.187 1.00 19.35	PROT
ATOM	815 CA PRO 323	56.462 -5.339 28.507 1.00 23.60	PROT
ATOM	816 CB PRO 323	56.390 -5.121 30.007 1.00 3.90	PROT
ATOM	817 CG PRO 323	55.031 -5.570 30.360 1.00 14.06	PROT
ATOM	818 C PRO 323	56.949 -6.736 28.151 1.00 21.79	PROT
ATOM	819 O PRO 323	58.149 -7.003 28.119 1.00 27.28	PROT
ATOM ATOM	820 N GLU 324 821 CA GLU 324	56.009 -7.633 27.889 1.00 37.63 56.366 -8.993 27.524 1.00 42.63	PROT
ATOM	821 CA GLU 324 822 CB GLU 324		PROT
ATOM	823 C GLU 324	55.133 -9.885 27.551 1.00 37.58 56.971 -8.956 26.124 1.00 43.28	PROT
ATOM	824 O GLU 324	58.154 -9.239 25.938 1.00 43.14	PROT PROT
ATOM	825 N SER 325	56.153 -8.586 25.142 1.00 31.72	PROT
ATOM	826 CA SER 325	56.607 -8.508 23,765 1.00 30.34	PROT
ATOM	827 CB SER 325	55.413 -8.522 22.814 1.00 17.63	PROT
ATOM	828 OG SER 325	54.356 -7.729 23.315 1.00 31.90	PROT
ATOM	829 C SER 325	57.441 -7.257 23.519 1.00 31.94	PROT
ATOM	830 O SER 325	58.146 -7.169 22.513 1.00 45.47	PROT
ATOM	831 N GLU 326	57.359 -6.289 24.429 1.00 31.10	PROT
ATOM	832 CA GLU 326	58.119 -5.050 24.281 1.00 31.43	PROT
ATOM	833 CB GLU 326	59.598 -5.382 24.091 1.00 30.39	PROT
ATOM	834 CG GLU 326	60.552 -4.342 24.612 1.00 35.00	PROT
ATOM	835 CD GLU 326	61.738 -4.965 25.304 1.00 29.12	PROT
ATOM	836 OE1 GLU 326	61.525 -5.579 26.370 1.00 39.21	PROT
ATOM	837 OE2 GLU 326	62.872 -4.844 24.788 1.00 29.11	PROT

ATOM	838 C GLU 326	57.605 -4.283 23.063 1.00 28.37	PROT
ATOM	839 O GLU 326	58.382 -3.677 22.321 1.00 26.51	PROT
ATOM	840 N THR 327	56.290 -4.301 22.873 1.00 23.71	PROT
ATOM	841 CA THR 327	55.674 -3.648 21.720 1.00 22.11	PROT
ATOM	842 CB THR 327	55.298 -4.705 20.652 1.00 28.08	PROT
ATOM	843 OG1 THR 327	54.226 -5.524 21.145 1.00 16.87	PROT
ATOM	844 CG2 THR 327	56.494 -5.597 20.340 1.00 24.03	PROT
ATOM	845 C THR 327	54.420 -2.824 22.046 1.00 22.42	PROT
ATOM	846 O THR 327	53.928 -2.830 23.172 1.00 17.50	PROT
ATOM	847 N LEU 328	53.914 -2.122 21.038 1.00 17.28	PROT
ATOM	848 CA LEU 328	52.728 -1.285 21.171 1.00 14.83	PROT
ATOM	849 CB LEU 328	53.065 0.157 20.806 1.00 15.27	PROT
ATOM	850 CG LEU 328	53.693 1.036 21.879 1.00 10.50	PROT
ATOM	851 CD1 LEU 328	54.137 2.336 21.254 1.00 16.75	PROT
ATOM	852 CD2 LEU 328	52.682 1.285 22.979 1.00 20.19	PROT
ATOM	853 C LEU 328	51.687 -1.804 20.198 1.00 18.16	PROT
ATOM	854 O LEU 328	52.035 -2.508 19.254 1.00 23.88	PROT
ATOM	855 N THR 329	50.421 -1.450 20.402 1.00 9.40	PROT
ATOM	856 CA THR 329	49.389 -1.920 19.495 1.00 8.26	PROT
ATOM	857 CB THR 329	48.460 -2.888 20.199 1.00 8.67	PROT
ATOM	858 OG1 THR 329	49.213 -4.052 20.577 1.00 13.23	PROT
ATOM	859 CG2 THR 329	47.308 -3.289 19.270 1.00 2.00	PROT
ATOM	860 C THR 329	48.569 -0.841 18.800 1.00 16.65	PROT
ATOM	861 O THR 329	47.726 -0.158 19.406 1.00 17.20	PROT
ATOM	862 N LEU 330	48.808 -0.725 17.495 1.00 21.56	PROT
ATOM	863 CA LEU 330	48.138 0.258 16.655 1.00 20.95	PROT
ATOM	864 CB LEU 330	49.106 0.676 15.539 1.00 17.36	PROT
ATOM	865 CG LEU 330	50.570 0.797 16.028 1.00 12.86	PROT
ATOM	866 CD1 LEU 330	51.531 0.521 14.898 1.00 10.10	PROT
ATOM	867 CD2 LEU 330	50.830 2.180 16.600 1.00 2.00	PROT
ATOM	868 C LEU 330	46.803 -0.258 16.097 1.00 21.35	PROT
ATOM	869 O LEU 330	46.655 -1.444 15.791 1.00 21.93	PROT
ATOM	870 N ASN 331	45.834 0.648 15.987 1.00 27.76	PROT
ATOM	871 CA ASN 331	44.487 0.338 15.498 1.00 28.09	PROT
ATOM	872 CB ASN 331	44.460 0.275 13.971 1.00 24.95	PROT
ATOM	873 CG ASN 331	43.074 0.540 13.397 1.00 33.45	PROT
ATOM	874 OD1 ASN 331	42.512 -0.305 12.701 1.00 38.21	PROT
ATOM ATOM	875 ND2 ASN 331	42.522 1.715 13.680 1.00 24.73	PROT
	876 C ASN 331	43.946 -0.967 16.075 1.00 32.03	PROT
ATOM	877 O ASN 331 878 N GLY 332	43.166 -1.668 15.431 1.00 35.49	PROT
ATOM		44.357 -1.282 17.299 1.00 40.24	PROT
ATOM ATOM	879 CA GLY 332 880 C GLY 332	43.894 -2.495 17.941 1.00 38.04	PROT
ATOM	880 C GLY 332 881 O GLY 332	44.009 -3.665 16.998 1.00 40.09 43.001 -4.225 16.563 1.00 45.79	PROT
ATOM	882 N GLU 333	43.001 -4.225 16.563 1.00 45.79 45.249 -4.013 16.664 1.00 41.60	PROT
ATOM		45.539 -5.126 15.763 1.00 36.28	PROT
ATOM	883 CA GLU 333	4J.JJJ -J.120 1J./05 1.00 30.28	PROT

ATOM	884 CB GLU 333	44.752 -4.978 14.454 1.00 46.39	PROT
ATOM	885 CG GLU 333	44.745 -3.580 13.862 1.00 58.03	PROT
ATOM	886 CD GLU 333	43.883 -3.485 12.610 1.00 67.00	PROT
ATOM	887 OE1 GLU 333	44.446 -3.282 11.511 1.00 67.51	PROT
ATOM	888 OE2 GLU 333	42.644 -3.615 12.727 1.00 71.01	PROT
ATOM	889 C-GLU 333	47.027 -5.266 15.446 1.00 33.13	PROT
ATOM	890 O GLU 333	47.563 -6.366 15.486 1.00 27.97	PROT
ATOM	891 N MET 334	47.692 -4.152 15.143 1.00 27.00	PROT
ATOM	892 CA MET 334	49.111 -4.188 14.798 1.00 29.83	PROT
ATOM	893 CB MET 334	49.416 -3.159 13.699 1.00 26.04	PROT
ATOM	894 CG MET 334	50.561 -3.588 12.765 1.00 28.06	PROT
ATOM	895 SD MET 334	51.263 -2.273 11.736 1.00 28.46	PROT
ATOM	896 CE MET 334	50.021 -2.123 10.497 1.00 22.48	PROT
ATOM	897 C MET 334	50.087 -3.995 15.959 1.00 33.52	PROT
ATOM	898 O MET 334	50.071 -2.962 16.631 1.00 35.81	PROT
ATOM	899 N ALA 335	50.942 -4.996 16.171 1.00 27.46	PROT
ATOM	900 CA ALA 335	51.948 -4.976 17.234 1.00 29.69	PROT
ATOM	901 CB ALA 335	51.966 -6.314 17.965 1.00 12.67	PROT
ATOM	902 C ALA 335	53.336 -4.682 16.662 1.00 31.74	PROT
ATOM	903 O ALA 335	53.943 -5.530 16.009 1.00 43.66	PROT
ATOM	904 N VAL 336	53.848 -3.489 16.923 1.00 23.98	PROT
ATOM	905 CA VAL 336	55.151 -3.118 16.405 1.00 21.32	PROT
ATOM	906 CB VAL 336	55.028 -1.873 15.504 1.00 17.37	PROT
ATOM	907 CG1 VAL 336	53.945 -2.104 14.462 1.00 14.88	PROT
ATOM	908 CG2 VAL 336	54.686 -0.648 16.339 1.00 15.53	PROT
ATOM	909 C VAL 336	56.150 -2.852 17.526 1.00 22.72	PROT
ATOM	910 O VAL 336	55.763 -2.540 18.651 1.00 25.15	PROT
ATOM	911 N THR 337	57.435 -3.001 17.220 1.00 19.21	PROT
ATOM	912 CA THR 337	58.476 -2.765 18.205 1.00 20.31	PROT
ATOM	913 CB THR 337	59.752 -3.578 17.884 1.00 14.76	PROT
ATOM	914 OG1 THR 337	59.957 -3.616 16.467 1.00 16.43	PROT
ATOM	915 CG2 THR 337	59.615 -4.995 18.393 1.00 7.08	PROT
ATOM	916 C THR 337	58.785 -1.272 18.157 1.00 24.20	PROT
ATOM	917 O THR 337	58.322 -0.591 17.245 1.00 28.05	PROT
ATOM	918 N ARG 338	59.548 -0.766 19:134 1.00 27.55	PROT
ATOM	919 CA ARG 338	59.917 0.655 19.197 1.00 16.80	PROT
ATOM	920 CB ARG 338	60.757 0.942 20.446 1.00 17.04	PROT
ATOM	921 CG ARG 338	61.687 2.149 20.303 1.00 9.79	PROT
ATOM	922 CD ARG 338	62.666 2.276 21.458 1.00 2.00	PROT
ATOM	923 NE ARG 338	61.994 2.128 22.739 1.00 20.70	PROT
ATOM	924 CZ ARG 338	61.897 3.083 23.657 1.00 12.04	PROT
ATOM	925 NH1 ARG 338	61.261 2.840 24.784 1.00 27.11	PROT
ATOM	926 NH2 ARG 338	62.436 4.272 23.459 1.00 22.23	PROT
ATOM	927 C ARG 338	60.702 1.085 17.968 1.00 21.26	PROT
ATOM	928 O ARG 338	60.338 2.049 17.295 1.00 16.40	PROT
ATOM	929 N GLY 339	61.792 0.374 17.693 1.00 31.57	PROT

ATOM	930 CA GLY 339	62.609 0.696 16.540 1.00 32.42	PROT
ATOM	931 C GLY 339	61.816 0.534 15.254 1.00 30.08	PROT
ATOM	932 O GLY 339	61.932 1.342 14.328 1.00 25.82	PROT
ATOM	933 N GLN 340	61.008 -0.520 15.192 1.00 16.60	PROT
ATOM	934 CA GLN 340	60.191 -0.768 14.012 1.00 14.08	PROT
ATOM	935 CB GLN 340	59.199 -1.884 14.301 1.00 5.73	PROT
ATOM	936 CG GLN 340	58.849 -2.697 13.100 1.00 16.15	PROT
ATOM	937 CD GLN 340	58.577 -4.141 13.442 1.00 22.46	PROT
ATOM	938 OE1 GLN 340	57.767 -4.450 14.316 1.00 30.45	PROT
ATOM	939 NE2 GLN 340	59.254 -5.040 12.749 1.00 34.19	PROT
ATOM	940 C GLN 340	59.452 0.521 13.632 1.00 22.07	PROT
ATOM	941 O GLN 340	59.707 1.103 12.576 1.00 21.13	PROT
ATOM	942 N LEU 341	58.561 0.976 14.518 1.00 27.88	PROT
ATOM	943 CA LEU 341	57.778 2.197 14.306 1.00 21.82	PROT
ATOM	944 CB LEU 341	56.813 2.418 15.483 1.00 10.20	PROT
ATOM	945 CG LEU 341	55.930 3.682 15.534 1.00 16.27	PROT
ATOM	946 CD1 LEU 341	54.777 3.618 14.518 1.00 13.27	PROT
ATOM	947 CD2 LEU 341	55.370 3.822 16.935 1.00 10.68	PROT
ATOM	948 C LEU 341	58.683 3.413 14.138 1.00 13.98	PROT
ATOM	949 O LEU 341	58.315 4.386 13.486 1.00 7.94	PROT
ATOM	950 N LYS 342	59.867 3.361 14.734 1.00 11.48	PROT
ATOM	951 CA LYS 342	60.804 4.465 14.613 1.00 17.77	PROT
ATOM	952 CB LYS 342	62.063 4.213 15.459 1.00 13.58	PROT
ATOM	953 CG LYS 342	63.219 5.173 15.140 1.00 13.27	PROT
ATOM	954 CD LYS 342	64.173 5.358 16.319 1.00 5.44	PROT
ATOM	955 CE LYS 342	64.500 6.829 16.546 1.00 5.47	PROT
ATOM	956 NZ LYS 342	65.721 7.019 17.388 1.00 4.98	PROT
ATOM	957 C LYS 342	61.184 4.579 13.141 1.00 19.97	PROT
ATOM	958 O LYS 342	60.939 5.595 12.501 1.00 20.34	PROT
ATOM	959 N ASN 343	61.764 3.510 12.605 1.00 26.88	PROT
ATOM	960 CA ASN 343	62.196 3.470 11.219 1.00 22.34	PROT
ATOM	961 CB ASN 343	62.829 2.123 10.929 1.00 4.80	PROT
ATOM	962 CG ASN 343	64.060 1.894 11.758 1.00 18.77	PROT
ATOM	963 OD1 ASN 343	64.755 2.848 12.117 1.00 14.12	PROT
ATOM	964 ND2 ASN 343	64.340 0.634 12.083 1.00 12.72	PROT
ATOM	965 C ASN 343	61.091 3.736 10.224 1.00 20.40	PROT
ATOM	966 O ASN 343	61.309 4.417 9.232 1.00 20.76	PROT
ATOM	967 N GLY 344	59.908 3.200 10.494 1.00 12.62	PROT
ATOM	968 CA GLY 344	58.775 3.382 9.603 1.00 6.27	PROT
ATOM	969 C GLY 344	58.229 4.796 9.451 1.00 14.56	PROT
ATOM ATOM	970 O GLY 344 971 N GLY 345	57.177 4.972 8.826 1.00 13.30 58.002 5.705 10.030 1.00 16.51	PROT
ATOM	971 N GL1 345 972 CA GLY 345	58.902 5.795 10.030 1.00 16.51	PROT
ATOM	972 CA GLY 345 973 C GLY 345	58.439 7.166 9.869 1.00 20.04	PROT
ATOM		58.248 8.112 11.046 1.00 25.64	PROT
		58.243 9.331 10.849 1.00 23.32	PROT
ATOM	975 N LEU 346	58.099 7.588 12.260 1.00 22.22	PROT

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ATOM		57.874 8.449 13.415 1.00 14.94	PROT
ATOM		57.070 7.700 14.474 1.00 3.92	PROT
ATOM	·	55.566 7.538 14.193 1.00 5.92	PROT
ATOM		54.938 6.796 15.355 1.00 2.00	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	54.884 8.885 13.973 1.00 2.00	PROT
ATOM	•	59.126 9.042 14.041 1.00 14.60	PROT
ATOM		59.102 10.153 14.554 1.00 17.36	PROT
ATOM		60.226 8.312 14.001 1.00 12.09	PROT
ATOM		61.455 8.828 14.581 1.00 15.62	PROT
ATOM		61.439 8.963 16.090 1.00 6.31	PROT
ATOM	986 O GLY 347	60.865 8.141 16.790 1.00 13.15	PROT
ATOM		62.076 10.011 16.592 1.00 13.74	PROT
ATOM		62.141 10.259 18.030 1.00 10.13	PROT
ATOM	 	62.757 11.646 18.342 1.00 9.26	PROT
ATOM		61.867 12.752 17.794 1.00 2.00	PROT
ATOM	991 CG2 VAL 348	62.942 11.802 19.836 1.00 2.00	PROT
ATOM	992 C VAL 348	60.763 10.216 18.650 1.00 6.61	PROT
ATOM	993 O VAL 348	60.619 10.066 19.862 1.00 3.12	PROT
ATOM	994 N VAL 349	59.746 10.358 17.816 1.00 5.51	PROT
ATOM	995 CA VAL 349	58.386 10.342 18.306 1.00 2.00	PROT
ATOM	996 CB VAL 349	57.421 10.886 17.260 1.00 4.46	PROT
ATOM	997 CG1 VAL 349	56.001 10.578 17.656 1.00 2.00	PROT
ATOM	998 CG2 VAL 349	57.623 12.387 17.122 1.00 2.00	PROT
ATOM	999 C VAL 349	57.995 8.933 18.687 1.00 9.15	PROT
ATOM	1000 O VAL 349	57.284 8.726 19.664 1.00 15.02	PROT
ATOM	1001 N SER 350	58.446 7.943 17.933 1.00 7.42	PROT
ATOM	1002 CA SER 350	58.087 6.590 18.315 1.00 12.87	PROT
ATOM	1003 CB SER 350	58.695 5.561 17.382 1.00 9.48	PROT
ATOM	1004 OG SER 350	58.529 4.269 17.931 1.00 10.82	PROT
ATOM	1005 C SER 350	58.628 6.364 19.717 1.00 15.55	PROT
ATOM	1006 O SER 350	57.963 5.761 20.558 1.00 25.88	PROT
ATOM	1007 N ASP 351	59.838 6.863 19.950 1.00 16.38	PROT
ATOM ATOM	1008 CA ASP 351 1009 CB ASP 351	60.522 6.743 21.230 1.00 9.58	PROT
ATOM		61.861 7.469 21.176 1.00 7.32	PROT
ATOM	1010 CG ASP 351 1011 OD1 ASP 351	62.989 6.576 20.742 1.00 24.16	PROT
ATOM	1011 OD1 ASP 351 1012 OD2 ASP 351	64.011 7.110 20.275 1.00 30.24 62.866 5.343 20.869 1.00 33.85	PROT
ATOM	1012 OD2 ASP 351 1013 C ASP 351	59.695 7.360 22.334 1.00 17.01	PROT
ATOM	1013 C ASP 351	59.605 6.822 23.435 1.00 17.01	PROT
ATOM	1014 O ASP 351 1015 N ALA 352	59.100 8.508 22.032 1.00 13.51	PROT
ATOM	1016 CA ALA 352	58.294 9.224 23.004 1.00 5.19	PROT
ATOM	1010 CA ALA 352	57.914 10.593 22.452 1.00 2.00	PROT
ATOM	1017 CB ALA 352	57.914 10.393 22.432 1.00 2.00	PROT
ATOM	1019 O ALA 352	56.701 8.360 24.535 1.00 7.20	PROT PROT
ATOM	1020 N ILE 353	56.396 7.832 22.393 1.00 7.20	PROT
	1021 CA ILE 353	55.201 7.049 22.677 1.00 5.90	PROT
111 0141	TOWN ON THE JUL	33.401 1.0 1 3 22.011 1.00 3.90	LVOI

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ATOM		54.468 6.626 21.381 1.00 5.87	PROT
ATOM		53.113 6.049 21.732 1.00 2.00	PROT
ATOM	1 1024 CG1 ILE 353	54.349 7.831 20.428 1.00 3.91	PROT
ATOM	1025 CD1 ILE 353	53.330 7.664 19.294 1.00 2.00	PROT
ATOM	1 1026 C ILE 353	55.554 5.795 23.484 1.00 12.46	PROT
ATOM		54.848 5.426 24.428 1.00 11.74	PROT
ATOM		56.644 5.131 23.122 1.00 19.57	PROT
ATOM		57.034 3.944 23.862 1.00 14.42	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	58.256 3.270 23.209 1.00 3.70	PROT
ATOM	· ·	57.890 2.141 22.284 1.00 9.42	PROT
ATOM		57.427 2.401 20.995 1.00 12.33	PROT
ATOM		57.912 0.822 22.727 1.00 15.63	PROT
ATOM		56.982 1.366 20.165 1.00 6.67	PROT
ATOM		57.468 -0.224 21.900 1.00 16.53	PROT
ATOM	· -	57.002 0.053 20.620 1.00 11.61	PROT
ATOM	1037 C PHE 354	57.322 4.346 25.307 1.00 18.55	PROT
ATOM	1038 O PHE 354	56.796 3.740 26.233 1.00 16.67	PROT
ATOM	1039 N ASP 355	58.125 5.392 25.491 1.00 12.83	PROT
ATOM	1040 CA ASP 355	58.486 5.881 26.818 1.00 5.31	PROT
ATOM	1041 CB ASP 355	59.351 7.132 26.697 1.00 9.38	PROT
ATOM	1042 CG ASP 355	60.805 6.814 26.428 1.00 5.96	PROT
ATOM	1043 OD1 ASP 355	61.112 5.683 26.016 1.00 8.53	PROT
ATOM	1044 OD2 ASP 355	61.650 7.706 26.628 1.00 15.51	PROT
ATOM	1045 C ASP 355	57.252 6.199 27.659 1.00 10.27	PROT
ATOM	1046 O ASP 355	57.231 5.972 28.871 1.00 21.86	PROT
ATOM	1047 N LEU 356	56.224 6.726 27.014 1.00 4.18	PROT
ATOM	1048 CA LEU 356	54.988 7.061 27.697 1.00 2.07	PROT
ATOM ATOM	1049 CB LEU 356 1050 CG LEU 356	54.086 7.865 26.771 1.00 2.24	PROT
ATOM		52.694 8.229 27.266 1.00 3.11	PROT
ATOM		52.771 9.317 28.323 1.00 2.00	PROT
ATOM		51.877 8.709 26.086 1.00 2.00 54.281 5.786 28.091 1.00 9.17	PROT
ATOM	1053 C LEU 356 1054 O LEU 356		PROT
ATOM	1055 N GLY 357	53.831 5.644 29.221 1.00 14.77 54.183 4.856 27.147 1.00 13.10	PROT
ATOM	1056 CA GLY 357	53.515 3.597 27.413 1.00 6.91	PROT
ATOM	1057 C GLY 357	54.113 2.879 28.598 1.00 8.33	PROT
ATOM	1058 O GLY 357	53.400 2.426 29.492 1.00 9.09	PROT
ATOM	1059 N MET 358	55.435 2.768 28.607 1.00 12.61	PROT PROT
ATOM	1060 CA MET 358	56.112 2.091 29.692 1.00 10.53	PROT
ATOM	1061 CB MET 358	57.626 2.153 29.498 1.00 5.45	PROT
ATOM	1062 CG MET 358	58.138 1.507 28.210 1.00 15.15	PROT
ATOM	1063 SD MET 358	59.971 1.352 28.113 1.00 17.63	PROT
ATOM	1064 CE MET 358	60.445 3.023 27.774 1.00 20.56	PROT
ATOM	1065 C MET 358	55.714 2.809 30.972 1.00 15.08	PROT
ATOM	1066 O MET 358	55.241 2.191 31.920 1.00 27.69	PROT
ATOM	1067 N SER 359	55.875 4.125 30.984 1.00 20.67	PROT
	TOTAL DESCRIPTION	55.575 T.125 JU.70T 1.00 20.07	LVOI

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ATOM		55.551 4.924 32.158 1.00 19.72	PROT
ATOM		55.831 6.398 31.861 1.00 19.98	PROT
ATOM	1070 OG SER 359	54.753 7.220 32.262 1.00 33.66	PROT
ATOM	1071 C SER 359	54.115 4.757 32.656 1.00 22.67	PROT
ATOM	1072 O SER 359	53.849 4.837 33.860 1.00 22.94	PROT
ATOM	1073 N LEU 360	53.197 4.514 31.727 1.00 20.55	PROT
ATOM	1074 CA LEU 360	51.785 4.360 32.054 1.00 17.01	PROT
ATOM	1075 CB LEU 360	50.934 4.578 30.802 1.00 2.60	PROT
ATOM	1076 CG LEU 360	50.674 5.988 30.291 1.00 6.99	PROT
ATOM	1077 CD1 LEU 360	49.589 5.935 29.236 1.00 4.15	PROT
ATOM	1078 CD2 LEU 360	50.247 6.892 31.432 1.00 18.93	PROT
ATOM	1079 C LEU 360	51.437 3.001 32.638 1.00 19.29	PROT
ATOM	1080 O LEU 360	50.319 2.802 33.102 1.00 27.53	PROT
ATOM	1081 N SER 361	52.375 2.061 32.596 1.00 21.73	PROT
ATOM	1082 CA SER 361	52.139 0.712 33.114 1.00 23.03	PROT
ATOM	1083 CB SER 361	53.415 -0.130 33.027 1.00 25.89	PROT
ATOM	1084 OG SER 361	53.645 -0.613 31.717 1.00 27.77	PROT
ATOM	1085 C SER 361	51.681 0.730 34.563 1.00 23.26	PROT
ATOM	1086 O SER 361	50.720 0.046 34.929 1.00 18.73	PROT
ATOM	1087 N SER 362	52.388 1.524 35.367 1.00 29.84	PROT
ATOM	1088 CA SER 362	52.141 1.668 36.799 1.00 24.49	PROT
ATOM	1089 CB SER 362	53.435 2.089 37.491 1.00 26.14	PROT
ATOM	1090 OG SER 362	53.917 3.305 36.949 1.00 25.03	PROT
ATOM	1091 C SER 362	51.031 2.635 37.210 1.00 26.86	PROT
ATOM	1092 O SER 362	50.797 2.831 38.404 1.00 39.63	PROT
ATOM	1093 N PHE 363	50.361 3.251 36.240 1.00 20.94	PROT
ATOM	1094 CA PHE 363	49.272 4.185 36.545 1.00 18.33	PROT
ATOM	1095 CB PHE 363	49.191 5.294 35.486 1.00 17.03	PROT
ATOM	1096 CG PHE 363	50.171 6.407 35.706 1.00 22.73	PROT
ATOM	1097 CD1 PHE 363	49.733 7.689 35.990 1.00 9.72	PROT
ATOM	1098 CD2 PHE 363	51.545 6.167 35.659 1.00 24.77	PROT
ATOM	1099 CE1 PHE 363	50.645 8.712 36.225 1.00 16.85	PROT
ATOM	1100 CE2 PHE 363	52.463 7.198 35.897 1.00 14.26	PROT
ATOM	1101 CZ PHE 363	52.011 8.462 36.179 1.00 2.26	PROT
ATOM	1102 C PHE 363	47.958 3.417 36,598 1.00 16.57	PROT
ATOM	1103 O PHE 363	46.971 3.882 37.165 1.00 13.08	PROT
ATOM	1104 N ASN 364	47.976 2.231 36.002 1.00 17.31	PROT
ATOM	1105 CA ASN 364	46.819 1.349 35.949 1.00 26.11	PROT
ATOM	1106 CB ASN 364	46.673 0.608 37.276 1.00 16.96	PROT
ATOM	1107 CG ASN 364	47.402 -0.715 37.267 1.00 31.34	PROT
ATOM	1108 OD1 ASN 364	46.965 -1.657 36.613 1.00 36.66	PROT
ATOM	1109 ND2 ASN 364	48.527 -0.794 37.985 1.00 31.61	PROT
ATOM	1110 C ASN 364	45.527 2.060 35.594 1.00 18.22	PROT
ATOM	1111 O ASN 364	44.522 1.923 36.286 1.00 23.17	PROT
ATOM	1112 N LEU 365	45.567 2.803 34.491 1.00 13.10	PROT
ATOM	1113 CA LEU 365	44.417 3.562 34.013 1.00 15.41	PROT

ATOM	I 1114 CB LEU 365	44.833 4.483 32.861 1.00 16.55	PROT
ATOM	1 1115 CG LEU 365	45.762 5.653 33.181 1.00 19.56	PROT
ATOM	1116 CD1 LEU 365	46.146 6.373 31.897 1.00 6.69	PROT
ATOM	1117 CD2 LEU 365	45.067 6.602 34.128 1.00 15.69	PROT
ATOM	1118 C LEU 365	43.328 2.624 33.520 1.00 12.07	PROT
ATOM	1119 O- LEU 365	43.620 1.534 33.043 1.00 19.81	PROT
ATOM	1120 N ASP 366	42.077 3.047 33.653 1.00 10.86	PROT
ATOM	1121 CA ASP 366	40.942 2.263 33.180 1.00 8.96	PROT
ATOM	1122 CB ASP 366	39.933 2.021 34.326 1.00 9.59	PROT
ATOM	1123 CG ASP 366	39.300 3.306 34.859 1.00 21.78	PROT
ATOM	1124 OD1 ASP 366	39.871 4.397 34.676 1.00 25.60	PROT
ATOM	1125 OD2 ASP 366	38.217 3.222 35.474 1.00 19.16	PROT
ATOM	1126 C ASP 366	40.288 3.005 32.002 1.00 8.82	PROT
ATOM	1127 O ASP 366	40.666 4.132 31.681 1.00 17.66	PROT
ATOM	1128 N ASP 367	39.321 2.379 31.346 1.00 9.45	PROT
ATOM	1129 CA ASP 367	38.668 3.023 30.218 1.00 11.11	PROT
ATOM	1130 CB ASP 367	37.457 2.205 29.769 1.00 20.67	PROT
ATOM	1131 CG ASP 367	37.832 0.812 29.301 1.00 25.02	PROT
ATOM	1132 OD1 ASP 367	39.040 0.525 29.158 1.00 21.06	PROT
ATOM	1133 OD2 ASP 367	36.909 0.002 29.076 1.00 31.37	PROT
ATOM	1134 C ASP 367	38.233 4.445 30.574 1.00 14.44	PROT
ATOM	1135 O ASP 367	38.457 5.380 29.815 1.00 26.42	PROT
ATOM	1136 N THR 368	37.619 4.612 31.735 1.00 13.62	PROT
ATOM	1137 CA THR 368	37.157 5.926 32.160 1.00 13.14	PROT
ATOM	1138 CB THR 368	36.510 5.853 33.547 1.00 16.53	PROT
ATOM	1139 OG1 THR 368	35.482 4.856 33.550 1.00 10.44	PROT
ATOM	1140 CG2 THR 368	35.928 7.188 33.925 1.00 5.20	PROT
ATOM	1141 C THR 368	38.291 6.942 32.226 1.00 13.03	PROT
ATOM	1142 O THR 368	38.114 8.108 31.878 1.00 12.90	PROT
ATOM	1143 N GLU 369	39.455 6.492 32.686 1.00 9.96	PROT
ATOM	1144 CA GLU 369	40.616 7.365 32.821 1.00 7.34	PROT
ATOM	1145 CB GLU 369	41.673 6.687 33.708 1.00 10.25	PROT
ATOM	1146 CG GLU 369	41.584 7.113 35.189 1.00 14.56	PROT
ATOM	1147 CD GLU 369	41.599 5.945 36.167 1.00 19.39	PROT
ATOM	1148 OE1 GLU 369	42.255 4.922 35.864 1.00 19.65	PROT
ATOM ATOM	1149 OE2 GLU 369 1150 C GLU 369	40.954 6.054 37.233 1.00 7.98	PROT
ATOM	1150 C GLU 369	41.203 7.768 31.468 1.00 4.33	PROT
ATOM	1151 O GLO 309 1152 N VAL 370	41.467 8.944 31.213 1.00 7.50 41.406 6.784 30.603 1.00 12.29	PROT
ATOM	1152 N VAL 370 1153 CA VAL 370	41.406 6.784 30.603 1.00 12.29 41.927 7.040 29.267 1.00 19.01	PROT
ATOM	1154 CB VAL 370	42.092 5.726 28.496 1.00 19.01	PROT PROT
ATOM	1155 CG1 VAL 370	42.431 6.011 27.049 1.00 8.57	PROT
ATOM	1156 CG2 VAL 370	43.168 4.877 29.159 1.00 8.37	PROT
ATOM	1150 CG2 VAL 370	40.896 7.915 28.555 1.00 18.30	PROT
ATOM	1158 O VAL 370	41.230 8.872 27.855 1.00 17.19	PROT
ATOM	1159 N ALA 371	39.633 7.581 28.760 1.00 2.00	PROT
1110111	III) IV ILLA JII	57.055 7.501 20.700 1.00 2.00	1101

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ATOM		38.549 8.321 28.157 1.00 3.53	PROT
ATOM		37.215 7.728 28.591 1.00 9.17	PROT
ATOM		38.603 9.797 28.529 1.00 9.97	PROT
ATOM		38.626 10.666 27.655 1.00 24.55	PROT
ATOM		38.633 10.082 29.831 1.00 14.85	PROT
ATOM		38.636 11.463 30.307 1.00 9.24	PROT
ATOM		38.480 11.501 31.830 1.00 8.83	PROT
ATOM		37.043 11.288 32.364 1.00 5.50	PROT
ATOM		37.036 10.338 33.553 1.00 2.02	PROT
ATOM		36.455 12.626 32.770 1.00 2.00	PROT
ATOM		39.867 12.218 29.870 1.00 10.17	PROT
ATOM		39.791 13.413 29.568 1.00 7.23	PROT
ATOM		40.996 11.510 29.825 1.00 13.10	PROT
ATOM	1173 CA LEU 373	42.270 12.078 29.399 1.00 2.00	PROT
ATOM		43.325 10.981 29.381 1.00 2.00	PROT
ATOM	1175 CG LEU 373	44.705 11.118 30.045 1.00 9.64	PROT
ATOM	1176 CD1 LEU 373	44.817 12.382 30.875 1.00 2.00	PROT
ATOM	1177 CD2 LEU 373	44.955 9.883 30.882 1.00 2.00	PROT
ATOM	1178 C LEU 373	42.026 12.602 27.987 1.00 6.58	PROT
ATOM	1179 O LEU 373	42.357 13.738 27.660 1.00 9.73	PROT
ATOM	1180 N GLN 374	41.401 11.763 27.165 1.00 9.45	PROT
ATOM	1181 CA GLN 374	41.076 12.097 25.785 1.00 2.00	PROT
ATOM	1182 CB GLN 374	40.382 10.914 25.121 1.00 2.00	PROT
ATOM	1183 CG GLN 374	41.332 9.896 24.537 1.00 2.00	PROT
ATOM	1184 CD GLN 374	40.630 8.641 24.095 1.00 2.00	PROT
ATOM	1185 OE1 GLN 374	41.261 7.622 23.855 1.00 8.01	PROT
ATOM	1186 NE2 GLN 374	39.316 8.705 23.989 1.00 2.00	PROT
ATOM ATOM	1187 C GLN 374 1188 O GLN 374	40.187 13.326 25.694 1.00 2.78	PROT
ATOM		40.427 14.213 24.875 1.00 13.91	PROT
ATOM		39.151 13.386 26.521 1.00 2.00	PROT
ATOM	1190 CA ALA 375 1191 CB ALA 375	38.261 14.546 26.505 1.00 2.00 27.128 14.248 27.489 1.00 2.07	PROT
ATOM	1192 C ALA 375	37.128 14.348 27.489 1.00 3.97 39.061 15.801 26.868 1.00 4.60	PROT
ATOM	1193 O ALA 375	38.881 16.864 26.274 1.00 8.82	PROT
ATOM	1194 N VAL 376	39.956 15.667 27.842 1.00 9.01	PROT PROT
ATOM	1195 CA VAL 376	40.772 16.790 28.267 1.00 7.36	PROT
ATOM	1196 CB VAL 376	41.669 16.401 29.467 1.00 2.30	PROT
ATOM	1197 CG1 VAL 376	42.597 17.532 29.839 1.00 2.00	PROT
ATOM	1198 CG2 VAL 376	40.801 16.076 30.646 1.00 9.15	PROT
ATOM	1199 C VAL 376	41.629 17.256 27.110 1.00 3.94	PROT
ATOM	1200 O VAL 376	41.788 18.455 26.880 1.00 2.00	PROT
ATOM	1201 N LEU 377	42.179 16.297 26.379 1.00 3.92	PROT
ATOM	1202 CA LEU 377	43.020 16.618 25.239 1.00 5.65	PROT
ATOM	1203 CB LEU 377	43.714 15.354 24.731 1.00 5.08	PROT
ATOM	1204 CG LEU 377	45.052 15.005 25.386 1.00 2.00	PROT
ATOM	1205 CD1 LEU 377	45.620 13.790 24.719 1.00 2.00	PROT
		20170 211717 1.00 2.00	11/01

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	ATOM	1206 CD2 LEU 377	46.016 16.157 25.264 1.00 4.14	PROT
	ATOM	1207 C LEU 377	42.173 17.271 24.137 1.00 11.35	PROT
	ATOM	1208 O LEU 377	42.607 18.240 23.515 1.00 8.78	PROT
	ATOM	1209 N LEU 378	40.959 16.766 23.912 1.00 5.62	PROT
	ATOM	1210 CA LEU 378	40.080 17.352 22.900 1.00 8.57	PROT
	ATOM	1211 CB LEU 378	38.784 16.553 22.788 1.00 5.98	PROT
	ATOM	1212 CG LEU 378	37.847 16.993 21.658 1.00 6.60	PROT
	ATOM	1213 CD1 LEU 378	38.550 16.826 20.329 1.00 2.00	PROT
	ATOM	1214 CD2 LEU 378	36.563 16.172 21.690 1.00 9.27	PROT
	ATOM	1215 C LEU 378	39.738 18.833 23.146 1.00 10.76	PROT
	ATOM	1216 O LEU 378	40.045 19.689 22.312 1.00 14.81	PROT
	ATOM	1217 N MET 379	39.106 19.139 24.278 1.00 13.15	PROT
	ATOM	1218 CA MET 379	38.735 20.521 24.591 1.00 13.60	PROT
	ATOM	1219 CB MET 379	37.698 20.543 25.709 1.00 12.57	PROT
	ATOM	1220 CG MET 379	36.425 19.782 25.395 1.00 21.12	PROT
	ATOM	1221 SD MET 379	35.533 20.396 23.927 1.00 15.79	PROT
	ATOM	1222 CE MET 379	34.397 19.099 23.756 1.00 13.95	PROT
	ATOM	1223 C MET 379	39.912 21.419 24.988 1.00 16.01	PROT
	ATOM	1224 O MET 379	39.981 21.897 26.121 1.00 16.95	PROT
	ATOM	1225 N SER 380	40.824 21.663 24.048 1.00 12.39	PROT
	ATOM	1226 CA SER 380	41.984 22.506 24.303 1.00 10.77	PROT
	ATOM	1227 CB SER 380	43.248 21.815 23.810 1.00 8.45	PROT
	ATOM	1228 OG SER 380	43.288 20.487 24.286 1.00 17.27	PROT
	ATOM	1229 C SER 380	41.825 23.859 23.621 1.00 15.58	PROT
	ATOM	1230 O SER 380	42.125 24.019 22.432 1.00 23.09	PROT
	ATOM	1231 N SER 381	41.368 24.837 24.396 1.00 23.65	PROT
	ATOM	1232 CA SER 381	41.123 26.187 23.904 1.00 25.18	PROT
	ATOM	1233 CB SER 381	40.449 27.018 25.003 1.00 34.78	PROT
	ATOM	1234 OG SER 381	41.250 27.073 26.170 1.00 37.79	PROT
	ATOM	1235 C SER 381	42.342 26.940 23.388 1.00 19.38	PROT
	ATOM	1236 O SER 381	42.216 28.032 22.850 1.00 28.81	PROT
	ATOM	1237 N ASP 382	43.519 26.361 23.523 1.00 11.80	PROT
	ATOM	1238 CA ASP 382	44.716 27.057 23.082 1.00 15.78	PROT
	ATOM	1239 CB ASP 382	45.908 26.595 23.909 1.00 33.97	PROT
	ATOM	1240 CG ASP 382	46.069 25.098 23.891 1.00 48.78	PROT
	ATOM	1241 OD1 ASP 382	45.169 24.401 24.406 1.00 45.58	PROT
	ATOM	1242 OD2 ASP 382	47.091 24.620 23.356 1.00 56.52	PROT
	ATOM	1243 C ASP 382	45.037 26.888 21.604 1.00 21.28	PROT
	ATOM	1244 O ASP 382	45.907 27.585 21.079 1.00 41.91	PROT
	ATOM	1245 N ARG 383	44.357 25.971 20.923 1.00 21.81	PROT
	ATOM	1246 CA ARG 383	44.636 25.773 19.503 1.00 18.95	PROT
	ATOM	1247 CB ARG 383	43.745 24.685 18.921 1.00 8.26	PROT
	ATOM	1248 CG ARG 383	43.580 23.491 19.821 1.00 18.07	PROT
	ATOM	1249 CD ARG 383	44.693 22.487 19.610 1.00 11.10	PROT
	ATOM	1250 NE ARG 383	44.480 21.261 20.378 1.00 20.54	PROT
4	ATOM	1251 CZ ARG 383	45.460 20.462 20.786 1.00 18.25	PROT

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ATOM		45.187 19.365 21.481 1.00 5.24	PROT
ATOM	1 1253 NH2 ARG 383	46.717 20.765 20.495 1.00 19.21	PROT
ATOM	1 1254 C ARG 383	44.420 27.064 18.728 1.00 19.64	PROT
ATOM	1 1255 O ARG 383	43.493 27.828 19.001 1.00 17.46	PROT
ATOM	1 1256 N PRO 384	45.298 27.342 17.762 1.00 25.37	PROT
ATOM	1257 CD PRO 384	46.485 26.567 17.359 1.00 35.06	PROT
ATOM	1258 CA PRO 384	45.124 28.569 16.983 1.00 27.53	PROT
ATOM	1259 CB PRO 384	46.422 28.693 16.181 1.00 18.75	PROT
ATOM	1260 CG PRO 384	47.041 27.338 16.190 1.00 27.78	PROT
ATOM	1261 C PRO 384	43.895 28.476 16.081 1.00 28.76	PROT
ATOM	1262 O PRO 384	43.562 27.402 15.560 1.00 31.18	PROT
ATOM	1263 N GLY 385	43.215 29.606 15.917 1.00 27.37	PROT
ATOM	1264 CA GLY 385	42.039 29.638 15.073 1.00 26.98	PROT
ATOM	1265 C GLY 385	40.728 29.442 15.803 1.00 27.46	PROT
ATOM	1266 O GLY 385	39.689 29.911 15.339 1.00 31.99	PROT
ATOM	1267 N LEU 386	40.756 28.756 16.939 1.00 34.99	PROT
ATOM	1268 CA LEU 386	39.524 28.515 17.673 1.00 37.24	PROT
ATOM	1269 CB LEU 386	39.820 27.947 19.059 1.00 26.60	PROT
ATOM	1270 CG LEU 386	40.233 26.472 18.988 1.00 32.45	PROT
ATOM	1271 CD1 LEU 386	40.177 25.859 20.363 1.00 34.82	PROT
ATOM	1272 CD2 LEU 386	39.314 25.719 18.030 1.00 29.64	PROT
ATOM	1273 C LEU 386	38.733 29.795 17.778 1.00 36.93	PROT
ATOM	1274 O LEU 386	39.291 30.881 17.674 1.00 37.60	PROT
ATOM	1275 N ALA 387	37.427 29.665 17.962 1.00 31.47	PROT
ATOM	1276 CA ALA 387	36.578 30.832 18.058 1.00 28.80	PROT
ATOM	1277 CB ALA 387	35.553 30.814 16.950 1.00 41.01	PROT
ATOM	1278 C ALA 387	35.890 30.864 19.400 1.00 28.89	PROT
ATOM	1279 O ALA 387	35.998 31.842 20.133 1.00 30.62	PROT
ATOM	1280 N CYS 388	35.167 29.797 19.710 1.00 25.92	PROT
ATOM	1281 CA CYS 388	34.469 29.712 20.978 1.00 26.90	PROT
ATOM	1282 CB CYS 388	33.224 28.823 20.826 1.00 21.38	PROT
ATOM	1283 SG CYS 388	31.625 29.732 20.698 1.00 33.66	PROT
ATOM	1284 C CYS 388	35.443 29.159 22.040 1.00 31.18	PROT
ATOM	1285 O CYS 388	35.272 28.054 22.552 1.00 36.57	PROT
ATOM	1286 N VAL 389	36.473 29.951 22.346 1.00 20.22	PROT
ATOM	1287 CA VAL 389	37.511 29.622 23.327 1.00 16.02	PROT
ATOM ATOM	1288 CB VAL 389	38.554 30.737 23.381 1.00 9.80	PROT
	1289 CG1 VAL 389	39.526 30.480 24.498 1.00 16.03	PROT
ATOM ATOM	1290 CG2 VAL 389 1291 C VAL 389	39.257 30.843 22.056 1.00 16.27	PROT
		36.977 29.425 24.753 1.00 18.85	PROT
ATOM ATOM	1292 O VAL 389 1293 N GLU 390	37.066 28.336 25.323 1.00 24.21 36.461 20.500 25.327 1.00 5.06	PROT
ATOM	1294 CA GLU 390	36.461 30.500 25.337 1.00 5.06 35.008 30.434 36.660 1.00 3.00	PROT
ATOM	•	35.908 30.434 26.660 1.00 2.00 35.002 31.684 26.052 1.00 5.13	PROT
ATOM	1295 CB GLU 390 1296 C GLU 390	35.092 31.684 26.952 1.00 5.13 35.047 29.184 26.817 1.00 3.75	PROT
ATOM	1297 O GLU 390		PROT
VIOM	1297 O GLU 390	35.252 28.419 27.754 1.00 23.35	PROT

ATOM	·	34.103 28.938 25.915 1.00 14.06	PROT
ATOM	1299 CA ARG 391	33.248 27.754 26.093 1.00 26.18	PROT
ATOM	1300 CB ARG 391	32.121 27.699 25.049 1.00 31.84	PROT
ATOM	1301 CG ARG 391	30.843 27.040 25.601 1.00 47.73	PROT
ATOM	1302 CD ARG 391	29.882 26.572 24.512 1.00 58.24	PROT
ATOM	1303 NE ARG 391	29.879 27.487 23.378 1.00 66.80	PROT
ATOM	1304 CZ ARG 391	29.001 28.470 23.211 1.00 69.56	PROT
ATOM	1305 NH1 ARG 391	29.088 29.255 22.139 1.00 66.99	PROT
ATOM	1306 NH2 ARG 391	28.034 28.663 24.105 1.00 56.08	PROT
ATOM	1307 C ARG 391	33.979 26.415 26.110 1.00 23.65	PROT
ATOM	1308 O ARG 391	33.561 25.479 26.794 1.00 28.58	PROT
ATOM	1309 N ILE 392	35.064 26.316 25.359 1.00 15.05	PROT
ATOM	1310 CA ILE 392	35.812 25.077 25.335 1.00 19.03	PROT
ATOM	1311 CB ILE 392	36.804 25.063 24.165 1.00 22.30	PROT
ATOM	1312 CG2 ILE 392	37.971 24.130 24.467 1.00 21.71	PROT
ATOM	1313 CG1 ILE 392	36.074 24.614 22.892 1.00 23.47	PROT
ATOM	1314 CD1 ILE 392	36.245 25.551 21.707 1.00 4.13	PROT
ATOM	1315 C ILE 392	36.544 24.907 26.671 1.00 25.03	PROT
ATOM	1316 O ILE 392	36.728 23.783 27.153 1.00 26.11	PROT
ATOM	1317 N GLU 393	36.947 26.029 27.266 1.00 30.74	PROT
ATOM	1318 CA GLU 393	37.630 26.021 28.558 1.00 23.39	PROT
ATOM	1319 CB GLU 393	38.073 27.430 28.930 1.00 27.18	PROT
ATOM	1320 CG GLU 393	39.435 27.817 28.402 1.00 41.39	PROT
ATOM	1321 CD GLU 393	39.990 29.051 29.093 1.00 47.72	PROT
ATOM	1322 OE1 GLU 393	39.365 29.524 30.070 1.00 39.94	PROT
ATOM	1323 OE2 GLU 393	41.051 29.547 28.653 1.00 51.17	PROT
ATOM	1324 C GLU 393	36.655 25.516 29.610 1.00 21.72	PROT
ATOM	1325 O GLU 393	36.942 24.574 30.344 1.00 22.82	PROT
ATOM	1326 N LYS 394	35.497 26.163 29.676 1.00 9.64	PROT
ATOM	1327 CA LYS 394	34.462 25.779 30.618 1.00 11.56	PROT
ATOM	1328 CB LYS 394	33.177 26.557 30.338 1.00 7.52	PROT
ATOM	1329 C LYS 394	34.213 24.280 30.492 1.00 16.31	PROT
ATOM	1330 O LYS 394	34.000 23.594 31.498 1.00 24.52	PROT
ATOM	1331 N TYR 395	34.251 23.763 29.264 1.00 12.79	PROT
ATOM	1332 CA TYR 395	34.033 22.332 29.057 1.00 19.02	PROT
ATOM	1333 CB TYR 395	33.803 22.025 27.572 1.00 27.90	PROT
ATOM	1334 CG TYR 395	32.454 22.456 27.027 1.00 31.64	PROT
ATOM	1335 CD1 TYR 395	32.136 22.267 25.684 1.00 30.15	PROT
ATOM	1336 CE1 TYR 395	30.927 22.695 25.160 1.00 28.34	PROT
ATOM	1337 CD2 TYR 395	31.514 23.085 27.835 1.00 34.21	PROT
ATOM	1338 CE2 TYR 395	30.298 23.518 27.317 1.00 34.01	PROT
ATOM	1339 CZ TYR 395	30.014 23.322 25.979 1.00 33.73	PROT
ATOM	1340 OH TYR 395	28.824 23.785 25.453 1.00 44.99	PROT
ATOM	1341 C TYR 395	35.208 21.490 29.584 1.00 19.03	PROT
ATOM	1342 O TYR 395	35.003 20.494 30.277 1.00 25.23	PROT
ATOM	1343 N GLN 396	36.437 21.883 29.256 1.00 17.76	PROT
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ATOM	1344 CA GLN 396	37.596 21.134 29.725 1.00 13.73	PROT
ATOM		38.905 21.766 29.240 1.00 2.45	PROT
ATOM	1346 CG GLN 396	40.061 20.767 29.110 1.00 2.00	PROT
ATOM		41.388 21.439 28.799 1.00 5.12	PROT
ATOM		41.706 22.484 29.359 1.00 10.11	PROT
ATOM	1349 NE2 GLN 396	42.169 20.840 27.903 1.00 9.09	PROT
ATOM		37.562 21.149 31.238 1.00 17.65	PROT
ATOM		37.802 20.125 31.894 1.00 9.63	PROT
ATOM	1352 N ASP 397	37.250 22.319 31.787 1.00 6.69	PROT
ATOM		37.178 22.476 33.226 1.00 9.36	PROT
ATOM	1354 CB ASP 397	36.732 23.893 33.570 1.00 11.44	PROT
ATOM	1355 CG ASP 397	37.867 24.891 33.446 1.00 18.32	PROT
ATOM	1356 OD1 ASP 397	39.033 24.438 33.397 1.00 24.00	PROT
ATOM	1357 OD2 ASP 397	37.615 26.114 33.395 1.00 20.67	PROT
ATOM	1358 C ASP 397	36.215 21.443 33.771 1.00 7.77	PROT
ATOM	1359 O ASP 397	36.497 20.771 34.761 1.00 7.66	PROT
ATOM	1360 N SER 398	35.087 21.293 33.093 1.00 9.19	PROT
ATOM	1361 CA SER 398	34.094 20.322 33.508 1.00 14.18	PROT
ATOM	1362 CB SER 398	32.916 20.334 32.542 1.00 12.11	PROT
ATOM	1363 OG SER 398	32.406 21.650 32.423 1.00 31.95	PROT
ATOM	1364 C SER 398	34.712 18.939 33.556 1.00 11.47	PROT
ATOM	1365 O SER 398	34.591 18.227 34.551 1.00 21.11	PROT
ATOM	1366 N PHE 399	35.394 18.565 32.485 1.00 18.68	PROT
ATOM	1367 CA PHE 399	36.017 17.252 32.417 1.00 24.93	PROT
ATOM	1368 CB PHE 399	36.587 17.012 31.014 1.00 23.38	PROT
ATOM	1369 CG PHE 399	35.543 16.705 29.981 1.00 20.19	PROT
ATOM	1370 CD1 PHE 399	35.224 17.638 28.997 1.00 22.94	PROT
ATOM	1371 CD2 PHE 399	34.878 15.486 29.988 1.00 8.62	PROT
ATOM	1372 CE1 PHE 399	34.257 17.361 28.029 1.00 12.53	PROT
ATOM	1373 CE2 PHE 399	33.914 15.201 29.027 1.00 19.25	PROT
ATOM	1374 CZ PHE 399	33.604 16.143 28.044 1.00 15.15	PROT
ATOM	1375 C PHE 399	37.113 17.097 33.463 1.00 23.06	PROT
ATOM	1376 O PHE 399	37.210 16.063 34.137 1.00 15.58	PROT
ATOM	1377 N LEU 400	37.932 18.131 33.604 1.00 22.12	PROT
ATOM	1378 CA LEU 400	39.017 18.095 34.567 1.00 18.27	PROT
ATOM	1379 CB LEU 400	39.846 19.372 34.461 1.00 10.06	PROT
ATOM	1380 CG LEU 400	41.021 19.248 33.491 1.00 8.13	PROT
ATOM	1381 CD1 LEU 400	41.616 20.594 33.195 1.00 2.00	PROT
ATOM	1382 CD2 LEU 400	42.055 18.333 34.095 1.00 13.73	PROT
ATOM	1383 C LEU 400	38.527 17.892 36.002 1.00 24.79	PROT
ATOM	1384 O LEU 400	39.189 17.228 36.787 1.00 26.46	PROT
ATOM	1385 N LEU 401	37.371 18.447 36.354 1.00 21.93	PROT
ATOM	1386 CA LEU 401	36.862 18.268 37.707 1.00 17.21	PROT
ATOM	1387 CB LEU 401	35.766 19.285 38.022 1.00 19.27	PROT
ATOM	1388 CG LEU 401	35.538 19.547 39.515 1.00 16.76	PROT
ATOM	1389 CD1 LEU 401	36.652 20.403 40.085 1.00 2.00	PROT

ATOM	· · · · · · · · · · · · · · · · · · ·	34.206 20.235 39.687 1.00 14.41	PROT
ATOM		36.316 16.864 37.879 1.00 18.03	PROT
ATOM		36.482 16.250 38.925 1.00 28.63	PROT
ATOM	·-·	35.656 16.346 36.856 1.00 9.30	PROT
ATOM	1394 CA ALA 402	35.124 15.000 36.951 1.00 7.03	PROT
ATOM	1395 CB ALA 402	34.233 14.703 35.758 1.00 14.15	PROT
ATOM	1396 C ALA 402	36.298 14.029 36.989 1.00 7.68	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	36.294 13.054 37.739 1.00 2.00	PROT
ATOM		37.311 14.305 36.178 1.00 4.49	PROT
ATOM	1399 CA PHE 403	38.477 13.439 36.140 1.00 9.18	PROT
ATOM	1400 CB PHE 403	39.510 13.977 35.138 1.00 12.80	PROT
ATOM	1401 CG PHE 403	40.545 12.957 34.693 1.00 5.42	PROT
ATOM	1402 CD1 PHE 403	41.590 13.334 33.859 1.00 2.00	PROT
ATOM	1403 CD2 PHE 403	40.480 11.634 35.103 1.00 2.00	PROT
ATOM	1404 CE1 PHE 403	42.546 12.410 33.448 1.00 2.00	PROT
ATOM	1405 CE2 PHE 403	41.440 10.711 34.688 1.00 2.00	PROT
ATOM	1406 CZ PHE 403	42.468 11.100 33.863 1.00 2.00	PROT
ATOM	1407 C PHE 403	39.080 13.366 37.539 1.00 10.08	PROT
ATOM	1408 O PHE 403	39.207 12.279 38.097 1.00 8.23	PROT
ATOM	1409 N GLU 404	39.451 14.514 38.103 1.00 12.64	PROT
ATOM	1410 CA GLU 404	40.030 14.546 39.448 1.00 19.23	PROT
ATOM	1411 CB GLU 404	40.227 15.989 39.942 1.00 19.80	PROT
ATOM	1412 CG GLU 404	41.532 16.220 40.728 1.00 24.03	PROT
ATOM	1413 CD GLU 404	41.474 17.429 41.655 1.00 29.60	PROT
ATOM	1414 OE1 GLU 404	41.706 18.565 41.182 1.00 29.51	PROT
ATOM	1415 OE2 GLU 404	41.197 17.247 42.861 1.00 30.42	PROT
ATOM	1416 C GLU 404	39.112 13.806 40.416 1.00 24.36	PROT
ATOM	1417 O GLU 404	39.571 12.963 41.200 1.00 28.04	PROT
ATOM	1418 N HIS 405	37.815 14.108 40.358 1.00 10.26	PROT
ATOM	1419 CA HIS 405	36.870 13.446 41.240 1.00 7.78	PROT
ATOM	1420 CB HIS 405	35.473 14.023 41.054 1.00 3.47	PROT
ATOM	1421 CG HIS 405	35.312 15.393 41.630 1.00 15.49	PROT
ATOM	1422 CD2 HIS 405	36.223 16.260 42.134 1.00 17.97	PROT
ATOM	1423 ND1 HIS 405	34.096 16.036 41.694 1.00 21.57	PROT
ATOM	1424 CE1 HIS 405	34.265 17.242 42.210 1.00 27.50	PROT
ATOM	1425 NE2 HIS 405	35.547 17.403 42.485 1.00 13.53	PROT
ATOM	1426 C HIS 405	36.856 11.936 41.005 1.00 14.88	PROT
ATOM	1427 O HIS 405	36.641 11.155 41.935 1.00 22.11	PROT
ATOM	1428 N TYR 406	37.091 11.512 39.767 1.00 16.52	PROT
ATOM	1429 CA TYR 406	37.085 10.083 39.491 1.00 14.35	PROT
ATOM	1430 CB TYR 406	37.007 9.808 37.989 1.00 9.90	PROT
ATOM	1431 CG TYR 406	36.840 8.346 37.657 1.00 2.00	PROT
ATOM	1432 CD1 TYR 406	35.587 7.742 37.676 1.00 8.84	PROT
ATOM	1433 CE1 TYR 406	35.433 6.382 37.386 1.00 8.78	PROT
ATOM	1434 CD2 TYR 406	37.939 7.562 37.338 1.00 15.34	PROT
ATOM	1435 CE2 TYR 406	37.801 6.204 37.044 1.00 13.48	PROT

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ATOM		36.548 5.624 37.073 1.00 15.64	PROT
ATOM		2.00	PROT
ATOM		38.340 9.466 40.071 1.00 9.54	PROT
ATOM		38.328 8.328 40.525 1.00 14.29	PROT
ATOM		39.430 10.217 40.058 1.00 6.56	PROT
ATOM		40.671 9.708 40.617 1.00 13.87	PROT
ATOM		41.808 10.728 40.474 1.00 11.28	PROT
ATOM	· · · · · · · · · · · · ·	42.902 10.413 41.461 1.00 6.25	PROT
ATOM	· 	42.357 10.714 39.039 1.00 18.73	PROT
ATOM	· · - ·	41.863 9.579 38.169 1.00 13.14	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	40.438 9.426 42.091 1.00 11.44	PROT
ATOM		40.691 8.325 42.571 1.00 4.46	PROT
ATOM	1448 N ASN 408	39.953 10.448 42.792 1.00 12.35	PROT
ATOM	1449 CA ASN 408	39.642 10.363 44.213 1.00 2.00	PROT
ATOM	1450 CB ASN 408	38.758 11.535 44.629 1.00 2.00	PROT
ATOM	1451 CG ASN 408	39.499 12.840 44.657 1.00 3.57	PROT
ATOM	1452 OD1 ASN 408	40.733 12.859 44.656 1.00 14.35	PROT
ATOM	1453 ND2 ASN 408	38.758 13.949 44.689 1.00 2.00	PROT
ATOM	1454 C ASN 408	38.868 9.078 44.432 1.00 6.49	PROT
ATOM	1455 O ASN 408	39.282 8.187 45.178 1.00 10.45	PROT
ATOM	1456 N TYR 409	37.731 8.987 43.766 1.00 2.00	PROT
ATOM	1457 CA TYR 409	36.900 7.816 43.893 1.00 9.20	PROT
ATOM	1458 CB TYR 409	35.879 7.783 42.760 1.00 11.66	PROT
ATOM	1459 CG TYR 409	35.121 6.489 42.683 1.00 12.54	PROT
ATOM	1460 CD1 TYR 409	33.984 6.281 43.456 1.00 29.23	PROT
ATOM	1461 CE1 TYR 409	33.285 5.077 43.403 1.00 25.45	PROT
ATOM	1462 CD2 TYR 409	35.547 5.465 41.850 1.00 24.96	PROT
ATOM	1463 CE2 TYR 409	34.860 4.259 41.788 1.00 33.40	PROT
ATOM	1464 CZ TYR 409	33.733 4.074 42.567 1.00 24.27	PROT
ATOM	1465 OH TYR 409	33.065 2.883 42.509 1.00 32.72	PROT
ATOM	1466 C TYR 409	37.753 6.553 43.867 1.00 13.96	PROT
ATOM	1467 O TYR 409	37.730 5.763 44.804 1.00 29.48	PROT
ATOM	1468 N ARG 410	38.531 6.399 42.803 1.00 23.04	PROT
ATOM	1469 CA ARG 410	39.377 5.230 42.588 1.00 22.09	PROT
ATOM	1470 CB ARG 410	39.982 5.327 41.190 1.00 13.24	PROT
ATOM	1471 CG ARG 410	38.947 5.399 40.090 1.00 14.01	PROT
ATOM	1472 CD ARG 410	38.934 4.111 39.275 1.00 16.49	PROT
ATOM	1473 NE ARG 410	40.227 3.848 38.651 1.00 9.77	PROT
ATOM	1474 CZ ARG 410	40.617 2.651 38.239 1.00 11.38	PROT
ATOM	1475 NH1 ARG 410	41.806 2.493 37.685 1.00 14.94	PROT
ATOM	1476 NH2 ARG 410	39.810 1.613 38.375 1.00 12.78	PROT
ATOM	1477 C ARG 410	40.486 4.914 43.604 1.00 24.49	PROT
ATOM	1478 O ARG 410	40.860 3.753 43.780 1.00 12.85	PROT
ATOM	1479 N LYS 411	41.023 5.931 44.262 1.00 24.16	PROT
ATOM	1480 CA LYS 411	42.085 5.706 45.235 1.00 27.14	PROT
ATOM	1481 CB LYS 411	41.525 5.069 46.516 1.00 37.40	PROT

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ATOM	. · · . · · · · · · · · · · · · · · · ·	40.317 5.779 47.103 1.00 35.00	PROT
ATOM		39.406 4.788 47.804 1.00 40.83	PROT
ATOM		38.414 5.496 48.725 1.00 58.04	PROT
ATOM	1 1485 NZ LYS 411	38.833 5.496 50.168 1.00 54.40	PROT
ATOM	1 1486 C LYS 411	43.186 4.814 44.664 1.00 28.02	PROT
ATOM	1 1487 O LYS 411	43.209 3.598 44.876 1.00 25.00	PROT
ATOM	1 1488 N HIS 412	44.091 5.438 43.923 1.00 30.05	PROT
ATOM	I 1489 CA HIS 412	45.223 4.738 43.332 1.00 26.70	PROT
ATOM	1 1490 CB HIS 412	45.756 5.491 42.104 1.00 29.28	PROT
ATOM	1 1491 CG HIS 412	44.953 5.289 40.857 1.00 18.44	PROT
ATOM	1 1492 CD2 HIS 412	43.783 5.836 40.451 1.00 19.98	PROT
ATOM	1 1493 ND1 HIS 412	45.366 4.465 39.833 1.00 16.33	PROT
ATOM	1494 CE1 HIS 412	44.486 4.513 38.850 1.00 24.80	PROT
ATOM	1495 NE2 HIS 412	43.516 5.338 39.200 1.00 23.01	PROT
ATOM	1496 C HIS 412	46.281 4.788 44.406 1.00 20.73	PROT
ATOM	1497 O HIS 412	46.335 5.740 45.171 1.00 24.69	PROT
ATOM	1498 N HIS 413	47.138 3.784 44.461 1.00 28.17	PROT
ATOM	1499 CA HIS 413	48.183 3.788 45.465 1.00 28.09	PROT
ATOM	1500 CB HIS 413	48.219 2.426 46.144 1.00 21.71	PROT
ATOM	1501 CG HIS 413	46.906 2.053 46.759 1.00 44.26	PROT
ATOM	1502 CD2 HIS 413	46.140 0.941 46.632 1.00 43.48	PROT
ATOM	1503 ND1 HIS 413	46.214 2.902 47.600 1.00 40.00	PROT
ATOM	1504 CE1 HIS 413	45.080 2.328 47.962 1.00 47.35	PROT
ATOM	1505 NE2 HIS 413	45.011 1.137 47.390 1.00 35.50	PROT
ATOM	1506 C HIS 413	49.527 4.194 44.875 1.00 26.49	PROT
ATOM	1507 O HIS 413	50.483 3.421 44.829 1.00 31.82	PROT
ATOM	1508 N VAL 414	49.555 5.439 44.411 1.00 18.32	PROT
ATOM	1509 CA VAL 414	50.726 6.069 43.820 1.00 22.60	PROT
ATOM	1510 CB VAL 414	50.718 5.966 42.290 1.00 32.50	PROT
ATOM	1511 CG1 VAL 414	51.636 7.026 41.694 1.00 33.83	PROT
ATOM	1512 CG2 VAL 414	51.169 4.574 41.863 1.00 40.20	PROT
ATOM	1513 C VAL 414	50.630 7.529 44.225 1.00 17.96	PROT
ATOM	1514 O VAL 414	49.708 8.236 43.829 1.00 30.33	PROT
ATOM	1515 N THR 415	51.586 7.969 45.028 1.00 32.51	PROT
ATOM	1516 CA THR 415	51.601 9.332 45.531 1.00 35.31	PROT
ATOM	1517 CB THR 415	52.779 9.529 46.511 1.00 49.75	PROT
ATOM	1518 OG1 THR 415	53.023 10.930 46.702 1.00 60.64	PROT
ATOM	1519 CG2 THR 415	54.038 8.850 45.974 1.00 50.83	PROT
ATOM	1520 C THR 415	51.668 10.387 44.436 1.00 31.44	PROT
ATOM	1521 O THR 415	52.423 10.251 43.475 1.00 22.01	PROT
ATOM	1522 N HIS 416	50.865 11.437 44.607 1.00 24.94	PROT
ATOM	1523 CA HIS 416	50.781 12.559 43.671 1.00 27.82	PROT
ATOM	1524 CB HIS 416	52.163 13.164 43.440 1.00 32.98	PROT
ATOM	1525 CG HIS 416	52.776 13.747 44.671 1.00 44.74	PROT
ATOM	1526 CD2 HIS 416	53.982 13.539 45.251 1.00 44.91	PROT
ATOM	1527 ND1 HIS 416	52.121 14.665 45.462 1.00 49.20	PROT

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ATOM	,	52.899 15.000 46.477 1.00 53.14	PROT
ATOM	1529 NE2 HIS 416	54.033 14.330 46.373 1.00 41.72	PROT
ATOM	1530 C HIS 416	50.176 12.172 42.328 1.00 29.13	PROT
ATOM	1531 O HIS 416	50.612 12.660 41.286 1.00 37.24	PROT
ATOM	1532 N PHE 417	49.163 11.311 42.350 1.00 18.38	PROT
ATOM	1533 CA PHE 417	48.528 10.867 41.115 1.00 16.08	PROT
ATOM		47.295 10.029 41.407 1.00 17.89	PROT
ATOM		47.021 8.997 40.364 1.00 16.15	PROT
ATOM		47.980 8.044 40.051 1.00 16.55	PROT
ATOM		45.806 8.971 39.696 1.00 15.49	PROT
ATOM	1538 CE1 PHE 417	47.727 7.081 39.087 1.00 19.81	PROT
ATOM		45.544 8.008 38.731 1.00 9.76	PROT
ATOM	1540 CZ PHE 417	46.501 7.064 38.427 1.00 5.25	PROT
ATOM	1541 C PHE 417	48.117 11.990 40.187 1.00 14.51	PROT
ATOM	1542 O PHE 417	48.636 12.119 39.081 1.00 18.44	PROT
ATOM	1543 N TRP 418	47.171 12.800 40.640 1.00 21.08	PROT
ATOM	1544 CA TRP 418	46.688 13.900 39.828 1.00 16.28	PROT
ATOM	1545 CB TRP 418	45.796 14.832 40.659 1.00 15.19	PROT
ATOM	1546 CG TRP 418	45.002 15.746 39.802 1.00 16.60	PROT
ATOM	1547 CD2 TRP 418	44.165 15.369 38.710 1.00 21.85	PROT
ATOM	1548 CE2 TRP 418	43.690 16.557 38.118 1.00 22.53	PROT
ATOM	1549 CE3 TRP 418	43.771 14.138 38.170 1.00 16.42	PROT
ATOM	1550 CD1 TRP 418	44.999 17.107 39.836 1.00 21.01	PROT
ATOM	1551 NE1 TRP 418	44.215 17.606 38.826 1.00 24.02	PROT
ATOM	1552 CZ2 TRP 418	42.838 16.555 37.010 1.00 24.64	PROT
ATOM	1553 CZ3 TRP 418	42.925 14.135 37.069 1.00 28.80	PROT
ATOM	1554 CH2 TRP 418	42.467 15.337 36.500 1.00 21.25	PROT
ATOM	1555 C TRP 418	47.834 14.676 39.192 1.00 16.17	PROT
ATOM	1556 O TRP 418	47.928 14.764 37.977 1.00 19.51	PROT
ATOM ATOM	1557 N PRO 419	48.723 15.250 40.007 1.00 19.59	PROT
	1558 CD PRO 419	48.757 15.274 41.477 1.00 19.81	PROT
ATOM ATOM	1559 CA PRO 419 1560 CB PRO 419	49.837 16.002 39.429 1.00 17.87	PROT
ATOM	1561 CG PRO 419	50.720 16.309 40.629 1.00 6.85	PROT
ATOM	1562 C PRO 419	49.785 16.326 41.764 1.00 25.11 50.578 15.202 38.373 1.00 15.44	PROT
ATOM	1563 O PRO 419	50.922 15.720 37.315 1.00 13.44	PROT
ATOM	1564 N LYS 420	50.811 13.932 38.664 1.00 15.10	PROT
ATOM	1565 CA LYS 420	51.534 13.056 37.748 1.00 20.59	PROT
ATOM	1566 CB LYS 420	51.900 11.746 38.471 1.00 28.85	PROT PROT
ATOM	1567 CG LYS 420	52.955 11.906 39.577 1.00 30.61	PROT
ATOM	1568 CD LYS 420	52.907 10.759 40.580 1.00 50.61	PROT
ATOM	1569 CE LYS 420	54.275 10.493 41.224 1.00 31.94	PROT
ATOM	1570 NZ LYS 420	54.485 9.040 41.557 1.00 27.34	PROT
ATOM	1571 C LYS 420	50.779 12.757 36.445 1.00 17.36	PROT
ATOM	1572 O LYS 420	51.393 12.439 35.437 1.00 26.28	PROT
ATOM	1573 N LEU 421	49.455 12.859 36.474 1.00 16.34	PROT
** 0141	15/5 IN LLU 721	77.700 12.007 JU.7/7 1.00 10.34	11/01

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ATOM	1574 CA LEU 421	48.627 12.614 35.297 1.00 9.38	PROT
ATOM	1575 CB LEU 421	47.231 12.139 35.707 1.00 13.22	PROT
ATOM	1576 CG LEU 421	46.739 10.818 35.107 1.00 15.75	PROT
ATOM	1577 CD1 LEU 421	47.919 9.993 34.652 1.00 29.24	PROT
ATOM	1578 CD2 LEU 421	45.949 10.049 36.135 1.00 12.19	PROT
ATOM	1579 C- LEU 421	48.511 13.866 34.441 1.00 12.61	PROT
ATOM	1580 O LEU 421	48.458 13.777 33.223 1.00 17.85	PROT
ATOM	1581 N LEU 422	48.451 15.036 35.063 1.00 8.47	PROT
ATOM	1582 CA LEU 422	48.393 16.254 34.277 1.00 7.21	PROT
ATOM	1583 CB LEU 422	48.160 17.468 35.164 1.00 2.00	PROT
ATOM	1584 CG LEU 422	46.941 17.445 36.088 1.00 12.16	PROT
ATOM	1585 CD1 LEU 422	47.024 18.660 36.982 1.00 6.96	PROT
ATOM	1586 CD2 LEU 422	45.632 17.450 35.313 1.00 2.00	PROT
ATOM	1587 C LEU 422	49.748 16.365 33.567 1.00 10.59	PROT
ATOM	1588 O LEU 422	49.851 16.938 32.477 1.00 13.48	PROT
ATOM	1589 N MET 423	50.786 15.804 34.185 1.00 2.29	PROT
ATOM	1590 CA MET 423	52.109 15.821 33.579 1.00 6.50	PROT
ATOM	1591 CB MET 423	53.158 15.215 34.514 1.00 2.13	PROT
ATOM	1592 CG MET 423	53.361 15.968 35.803 1.00 16.33	PROT
ATOM	1593 SD MET 423	55.075 16.415 36.070 1.00 26.66	PROT
ATOM	1594 CE MET 423	55.751 14.880 36.623 1.00 20.24	PROT
ATOM	1595 C MET 423	52.016 14.966 32.318 1.00 12.20	PROT
ATOM	1596 O MET 423	52.741 15.183 31.345 1.00 18.67	PROT
ATOM	1597 N LYS 424	51.114 13.988 32.352 1.00 7.89	PROT
ATOM	1598 CA LYS 424	50.907 13.084 31.230 1.00 12.91	PROT
ATOM	1599 CB LYS 424	49.990 11.924 31.645 1.00 5.14	PROT
ATOM	1600 CG LYS 424	50.669 10.579 31.980 1.00 11.76	PROT
ATOM	1601 CD LYS 424	52.187 10.590 31.866 1.00 3.70	PROT
ATOM	1602 CE LYS 424	52.844 10.020 33.113 1.00 7.84	PROT
ATOM	1603 NZ LYS 424	54.335 9.959 32.995 1.00 25.86	PROT
ATOM ATOM	1604 C LYS 424	50.293 13.840 30.046 1.00 17.44	PROT
ATOM	1605 O LYS 424 1606 N VAL 425	50.650 13.596 28.897 1.00 11.72	PROT
ATOM	1607 CA VAL 425	49.370 14.756 30.322 1.00 3.16	PROT
ATOM	1608 CB VAL 425	48.768 15.515 29.249 1.00 2.00 47.744 16.532 29.773 1.00 6.77	PROT
ATOM	1609 CG1 VAL 425	47.653 17.716 28.815 1.00 2.00	PROT
ATOM	1610 CG2 VAL 425	46.381 15.870 29.914 1.00 10.91	PROT
ATOM	1611 C VAL 425	49.845 16.274 28.487 1.00 4.83	PROT PROT
ATOM	1612 O VAL 425	49.853 16.265 27.269 1.00 15.69	PROT
ATOM	1613 N THR 426	50.753 16.924 29.208 1.00 14.38	PROT
ATOM	1614 CA THR 426	51.824 17.707 28.593 1.00 12.41	PROT
ATOM	1615 CB THR 426	52.713 18.372 29.667 1.00 12.49	PROT
ATOM	1616 OG1 THR 426	51.890 19.138 30.552 1.00 11.06	PROT
ATOM	1617 CG2 THR 426	53.763 19.283 29.015 1.00 2.93	PROT
ATOM	1618 C THR 426	52.734 16.928 27.653 1.00 15.72	PROT
ATOM	1619 O THR 426	53.198 17.463 26.651 1.00 14.40	PROT
	TAU	20.270 27.102 20.031 1.00 17.70	11.01

	ATOM	1620 N ASP 427	53.000 15.672 27.981 1.00 16.23	PROT
	ATOM	1621 CA ASP 427	53.865 14.843 27.157 1.00 16.35	PROT
	ATOM	1622 CB ASP 427	54.342 13.630 27.950 1.00 19.48	PROT
	ATOM	1623 CG ASP 427	55.337 13.997 29.029 1.00 18.96	PROT
	ATOM	1624 OD1 ASP 427	55.874 15.125 29.010 1.00 8.75	PROT
	ATOM	1625 OD2 ASP 427	55.579 13.145 29.902 1.00 24.25	PROT
	ATOM	1626 C ASP 427	53.155 14.381 25.891 1.00 20.52	PROT
	ATOM	1627 O ASP 427	53.793 14.164 24.856 1.00 25.69	PROT
	ATOM	1628 N LEU 428	51.838 14.218 25.986 1.00 5.49	PROT
	ATOM	1629 CA LEU 428	51.040 13.815 24.849 1.00 2.00	PROT
	ATOM	1630 CB LEU 428	49.634 13.470 25.301 1.00 2.00	PROT
	ATOM	1631 CG LEU 428	49.579 12.127 26.028 1.00 2.00	PROT
	ATOM	1632 CD1 LEU 428	48.184 11.789 26.481 1.00 2.00	PROT
	ATOM	1633 CD2 LEU 428	50.088 11.080 25.108 1.00 2.00	PROT
	ATOM	1634 C LEU 428	51.019 14.987 23.881 1.00 7.72	PROT
	ATOM	1635 O LEU 428	51.072 14.800 22.666 1.00 9.22	PROT
	ATOM	1636 N ARG 429	50.961 16.197 24.432 1.00 10.07	PROT
	ATOM	1637 CA ARG 429	50.948 17.438 23.659 1.00 7.97	PROT
	ATOM	1638 CB ARG 429	50.799 18.642 24.583 1.00 18.55	PROT
	ATOM	1639 CG ARG 429	49.548 18.634 25.429 1.00 14.80	PROT
	ATOM	1640 CD ARG 429	48.588 19.674 24.935 1.00 32.08	PROT
	ATOM	1641 NE ARG 429	47.508 19.923 25.880 1.00 42.46	PROT
	ATOM	1642 CZ ARG 429	46.226 19.673 25.631 1.00 48.51	PROT
	ATOM ATOM	1643 NH1 ARG 429 1644 NH2 ARG 429	45.860 19.163 24.459 1.00 33.35	PROT
	ATOM	1644 NH2 ARG 429 1645 C ARG 429	45.307 19.955 26.549 1.00 46.08 52.260 17.557 22.919 1.00 11.77	PROT
	ATOM	1646 O ARG 429		PROT
	ATOM	1647 N MET 430	52.298 17.904 21.737 1.00 28.66 53.343 17.270 23.629 1.00 20.26	PROT
	ATOM	1648 CA MET 430	54.671 17.328 23.042 1.00 21.06	PROT PROT
	ATOM	1649 CB MET 430	55.738 17.015 24.100 1.00 30.24	PROT
	ATOM	1650 CG MET 430	56.061 18.165 25.056 1.00 34.66	PROT
	ATOM	1651 SD MET 430	55.727 19.795 24.373 1.00 35.91	PROT
	ATOM	1652 CE MET 430	56.839 19.814 22.978 1.00 32.52	PROT
	ATOM	1653 C MET 430	54.735 16.302 21.925 1.00 18.70	PROT
	ATOM	1654 O MET 430	55.287 16.560 29.860 1.00 16.59	PROT
	ATOM	1655 N ILE 431	54.161 15.133 22.182 1.00 15.38	PROT
	ATOM	1656 CA ILE 431	54.144 14.069 21.196 1.00 15.85	PROT
	ATOM	1657 CB ILE 431	53.326 12.859 21.705 1.00 13.76	PROT
	ATOM	1658 CG2 ILE 431	52.727 12.084 20.539 1.00 11.11	PROT
	ATOM	1659 CG1 ILE 431	54.239 11.924 22.489 1.00 11.72	PROT
	ATOM	1660 CD1 ILE 431	53.552 11.224 23.615 1.00 16.22	PROT
	ATOM	1661 C ILE 431	53.538 14.609 19.904 1.00 18.49	PROT
	ATOM	1662 O ILE 431	54.134 14.483 18.839 1.00 17.36	PROT
	ATOM	1663 N GLY 432	52.361 15.220 20.003 1.00 2.00	PROT
	ATOM	1664 CA GLY 432	51.721 15.772 18.831 1.00 2.00	PROT
4	ATOM	1665 C GLY 432	52.542 16.851 18.148 1.00 10.55	PROT

ATOM	· · · · · · · · · · · · · · · · · · ·	52.707 16.834 16.936 1.00 9.60	PROT
ATOM	I 1667 N ALA 433	53.043 17.805 18.926 1.00 11.17	PROT
ATOM	1 1668 CA ALA 433	53.855 18.884 18.385 1.00 2.00	PROT
ATOM		54.326 19.771 19.506 1.00 2.00	PROT
ATOM	1670 C ALA 433	55.050 18.285 17.646 1.00 6.43	PROT
ATOM	1671 O- ALA 433	55.493 18.789 16.623 1.00 11.71	PROT
ATOM		55.579 17.197 18.179 1.00 15.71	PROT
ATOM		56.715 16.534 17.573 1.00 13.44	PROT
ATOM		57.228 15.464 18.518 1.00 14.76	PROT
ATOM		58.910 15.703 18.985 1.00 20.82	PROT
ATOM		56.269 15.902 16.264 1.00 9.28	PROT
ATOM		56.969 15.948 15.256 1.00 8.50	PROT
ATOM		55.091 15.300 16.298 1.00 11.04	PROT
ATOM		54.533 14.657 15.122 1.00 11.30	PROT
ATOM	1680 CB HIS 435	53.142 14.132 15.438 1.00 4.30	PROT
ATOM		52.480 13.460 14.283 1.00 13.68	PROT
ATOM	1682 CD2 HIS 435	52.751 12.288 13.662 1.00 4.72	PROT
ATOM	1683 ND1 HIS 435	51.358 13.976 13.666 1.00 5.53	PROT
ATOM	1684 CE1 HIS 435	50.966 13.147 12.717 1.00 12.84	PROT
ATOM	1685 NE2 HIS 435	51.794 12.116 12.694 1.00 15.77	PROT
ATOM	1686 C HIS 435	54.482 15.661 13.973 1.00 8.50	PROT
ATOM	1687 O HIS 435	54.941 15.370 12.869 1.00 14.82	PROT
ATOM	1688 N ALA 436	53.938 16.844 14.245 1.00 5.74	PROT
ATOM	1689 CA ALA 436	53.843 17.905 13.252 1.00 2.00	PROT
ATOM	1690 CB ALA 436	53.632 19.241 13.942 1.00 2.00	PROT
ATOM	1691 C ALA 436	55.121 17.934 12.406 1.00 8.68	PROT
ATOM	1692 O ALA 436	55.080 17.712 11.193 1.00 15.14	PROT
ATOM	1693 N SER 437	56.256 18.189 13.047 1.00 6.82	PROT
ATOM	1694 CA SER 437	57.522 18.226 12.337 1.00 9.05	PROT
ATOM	1695 CB SER 437 1696 OG SER 437	58.671 18.511 13.295 1.00 2.00	PROT
ATOM ATOM	· · · · · · · · · · · · · · · · · · ·	59.593 19.406 12.699 1.00 21.18	PROT
ATOM	1697 C SER 437 1698 O SER 437	57.758 16.896 11.637 1.00 15.18 58.076 16.849 10.445 1.00 19.33	PROT
ATOM	1699 N ARG 438	57.607 15.805 12.373 1.00 16.98	PROT
ATOM	1700 CA ARG 438	57.799 14.501 11.766 1.00 16.98	PROT
ATOM	1701 CB ARG 438	57.294 13.409 12.702 1.00 24.77	PROT PROT
ATOM	1701 CD ARG 438	58.006 12.086 12.534 1.00 33.76	PROT
ATOM	1703 CD ARG 438	59.506 12.280 12.614 1.00 30.64	PROT
ATOM	1704 NE ARG 438	60.219 11.380 11.721 1.00 29.76	PROT
ATOM	1705 CZ ARG 438	61.505 11.504 11.423 1.00 25.21	PROT
ATOM	1706 NH1 ARG 438	62.077 10.641 10.603 1.00 39.58	PROT
ATOM	1707 NH2 ARG 438	62.217 12.492 11.942 1.00 14.13	PROT
ATOM	1707 KHZ ARG 438	57.031 14.441 10.448 1.00 16.49	PROT
ATOM	1709 O ARG 438	57.563 14.008 9.424 1.00 15.57	PROT
ATOM	1710 N PHE 439	55.781 14.893 10.484 1.00 16.75	PROT
ATOM	1711 CA PHE 439	54.933 14.878 9.303 1.00 21.63	PROT
	TUY	2 2 2 1.00 21.03	1101

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ATOM	1712 CB PHE 439	53.603 15.575 9.574 1.00 17.84	PROT
ATOM	1713 CG PHE 439	52.597 15.364 8.490 1.00 20.60	PROT
ATOM	1714 CD1 PHE 439	52.042 14.103 8.279 1.00 30.60	PROT
ATOM	1715 CD2 PHE 439	52.265 16.394 7.622 1.00 14.95	PROT
ATOM	1716 CE1 PHE 439	51.175 13.867 7.206 1.00 29.12	PROT
ATOM	1717 CE2 PHE 439	51.404 16.173 6.552 1.00 25.18	PROT
ATOM	1718 CZ PHE 439	50.860 14.905 6.341 1.00 27.82	PROT
ATOM	1719 C PHE 439	55.620 15.548 8.130 1.00 28.17	PROT
ATOM	1720 O PHE 439	55.512 15.095 6.987 1.00 28.83	PROT
ATOM	1721 N LEU 440	56.328 16.633 8.427 1.00 26.77	PROT
ATOM	1722 CA LEU 440	57.055 17.382 7.418 1.00 24.66	PROT
ATOM	1723 CB LEU 440	57.555 18.696 8.005 1.00 10.80	PROT
ATOM	1724 CG LEU 440	56.501 19.658 8.541 1.00 8.60	PROT
ATOM	1725 CD1 LEU 440	57.152 20.985 8.855 1.00 17.69	PROT
ATOM	1726 CD2 LEU 440	55.410 19.847 7.522 1.00 15.71	PROT
ATOM	1727 C LEU 440	58.245 16.578 6.912 1.00 29.61	PROT
ATOM	1728 O LEU 440	58.506 16.526 5.718 1.00 32.37	PROT
ATOM	1729 N HIS 441	58.971 15.954 7.830 1.00 28.12	PROT
ATOM	1730 CA HIS 441	60.140 15.172 7.460 1.00 28.51	PROT
ATOM	1731 CB HIS 441	60.783 14.564 8.705 1.00 36.77	PROT
ATOM	1732 C HIS 441	59.724 14.081 6.497 1.00 31.94	PROT
ATOM	1733 O HIS 441	60.461 13.725 5.579 1.00 49.29	PROT
ATOM	1734 N MET 442	58.533 13.545 6.711 1.00 41.16	PROT
ATOM	1735 CA MET 442	58.033 12.487 5.854 1.00 39.99	PROT
ATOM	1736 CB MET 442	56.871 11.776 6.551 1.00 38.32	PROT
ATOM	1737 CG MET 442	57.263 11.122 7.860 1.00 19.20	PROT
ATOM	1738 SD MET 442	55.859 10.350 8.675 1.00 38.06	PROT
ATOM	1739 CE MET 442	54.906 11.767 9.073 1.00 21.45	PROT
ATOM	1740 C MET 442	57.599 13.031 4.495 1.00 35.68	PROT
ATOM	1741 O MET 442	57.887 12.431 3.461 1.00 27.43	PROT
ATOM	1742 N LYS 443	56.920 14.175 4.503 1.00 34.17	PROT
ATOM	1743 CA LYS 443	56.447 14.796 3.268 1.00 34.33	PROT
ATOM	1744 CB LYS 443	55.767 16.129 3.574 1.00 21.68	PROT
ATOM	1745 CG LYS 443	54.303 15.989 3.953 1.00 26.95	PROT
ATOM	1746 CD LYS 443	53.497 17.231 3.602 1.00 30.78	PROT
ATOM	1747 CE LYS 443	52.204 16.848 2.861 1.00 56.06	PROT
ATOM	1748 NZ LYS 443	50.931 17.261 3.564 1.00 45.26	PROT
ATOM	1749 C LYS 443	57.570 15.007 2.251 1.00 37.81	PROT
ATOM	1750 O LYS 443	57.325 15.049 1.041 1.00 38.26	PROT
ATOM	1751 N VAL 444	58.798 15.130 2.741 1.00 25.12	PROT
ATOM	1752 CA VAL 444	59.942 15.318 1.867 1.00 25.43	PROT
ATOM	1753 CB VAL 444	60.802 16.531 2.334 1.00 29.15	PROT
ATOM	1754 CG1 VAL 444	59.893 17.621 2.861 1.00 29.48	PROT
ATOM	1755 CG2 VAL 444	61.785 16.121 3.419 1.00 36.65	PROT
ATOM	1756 C VAL 444	60.786 14.042 1.825 1.00 30.03	PROT
ATOM	1757 O VAL 444	62.009 14.099 1.698 1.00 39.43	PROT

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ATOM	· · · · · · · · · · · · · · · · · · ·	60.127 12.888 1.903 1.00 39.84	PROT
ATOM		60.842 11.612 1.896 1.00 43.07	PROT
ATOM		61.429 11.360 3.282 1.00 50.55	PROT
ATOM	1761 CG GLU 445	62.399 10.203 3.351 1.00 77.00	PROT
ATOM		63.569 10.495 4.267 1.00 98.21	PROT
ATOM	1763 OE1 GLU 445	64.251 9.538 4.701 1.00100.00	PROT
ATOM	1764 OE2 GLU 445	63.804 11.690 4.554 1.00100.00	PROT
ATOM	1765 C GLU 445	59.989 10.408 1.491 1.00 43.41	PROT
ATOM	1766 O GLU 445	60.466 9.274 1.511 1.00 48.80	PROT
ATOM	1767 N CYS 446	58.731 10.644 1.137 1.00 38.17	PROT
ATOM	1768 CA CYS 446	57.852 9.548 0.743 1.00 41.38	PROT
ATOM	1769 CB CYS 446	57.066 9.035 1.965 1.00 40.61	PROT
ATOM	1770 SG CYS 446	58.062 8.276 3.320 1.00 44.73	PROT
ATOM	1771 C CYS 446	56.886 10.003 -0.362 1.00 45.83	PROT
ATOM	1772 O CYS 446	56.466 11.184 -0.323 1.00 44.17	PROT
ATOM	1773 OT CYS 446	56.570 9.180 -1.259 1.00 40.79	PROT
ATOM	1774 CB GLU 449	52.635 12.140 -2.649 1.00 28.60	PROT
ATOM	1775 C GLU 449	52.019 10.014 -1.526 1.00 38.06	PROT
ATOM	1776 O GLU 449	50.873 10.220 -1.935 1.00 43.52	PROT
ATOM	1777 N GLU 449	54.378 10.460 -2.167 1.00 17.78	PROT
ATOM	1778 CA GLU 449	53.105 11.069 -1.689 1.00 33.80	PROT
ATOM	1779 N LEU 450	52.387 8.880 -0.936 1.00 46.88	PROT
ATOM	1780 CA LEU 450	51.432 7.808 -0.696 1.00 52.62	PROT
ATOM	1781 CB LEU 450	52.101 6.436 -0.850 1.00 57.50	PROT
ATOM	1782 CG LEU 450	53.338 6.066 -0.028 1.00 59.81	PROT
ATOM	1783 CD1 LEU 450	53.613 4.573 -0.198 1.00 51.33	PROT
ATOM	1784 CD2 LEU 450	54.544 6.890 -0.473 1.00 57.03	PROT
ATOM	1785 C LEU 450	50.850 7.970 0.711 1.00 50.65	PROT
ATOM	1786 O LEU 450	50.965 7.091 1.569 1.00 38.49	PROT
ATOM	1787 N PHE 451	50.225 9.123 0.923 1.00 32.24	PROT
ATOM	1788 CA PHE 451	49.602 9.478 2.188 1.00 32.64	PROT
ATOM	1789 CB PHE 451	50.091 10.857 2.648 1.00 56.06	PROT
ATOM	1790 CG PHE 451	51.534 10.895 3.056 1.00 61.73	PROT
ATOM	1791 CD1 PHE 451	52.523 10.366 2.235 1.00 66.92	PROT
ATOM	1792 CD2 PHE 451	51.905 11.486 4.256 1.00 58.76	PROT
ATOM	1793 CE1 PHE 451	53.860 10.430 2.604 1.00 69.17	PROT
ATOM	1794 CE2 PHE 451	53.231 11.556 4.635 1.00 61.48	PROT
ATOM	1795 CZ PHE 451	54.214 11.028 3.809 1.00 71.95	PROT
ATOM	1796 C PHE 451	48.081 9.548 2.025 1.00 30.67	PROT
ATOM	1797 O PHE 451	47.571 10.429 1.324 1.00 38.49	PROT
ATOM	1798 N PRO 452	47.336 8.627 2.672 1.00 19.14	PROT
ATOM	1799 CD PRO 452	47.774 7.495 3.510 1.00 24.21	PROT
ATOM	1800 CA PRO 452	45.881 8.672 2.538 1.00 5.88	PROT
ATOM	1801 CB PRO 452	45.397 7.742 3.633 1.00 16.92	PROT
ATOM	1802 CG PRO 452	46.496 6.737 3.761 1.00 16.91	PROT
ATOM	1803 C PRO 452	45.354 10.090 2.687 1.00 15.15	PROT

ATOM	1 1804 O PRO 452	45.879 10.886 3.463 1.00 22.59	PROT
ATOM	I 1805 N PRO 453	44.315 10.429 1.920 1.00 18.37	PROT
ATOM		43.653 9.540 0.951 1.00 3.83	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	43.710 11.766 1.960 1.00 14.00	PROT
ATOM	1 1808 CB PRO 453	42.502 11.649 1.032 1.00 20.04	PROT
ATOM		42.316 10.163 0.807 1.00 19.43	PROT
ATOM	1810 C PRO 453	43.321 12.277 3.346 1.00 14.70	PROT
ATOM		43.609 13.422 3.682 1.00 9.70	PROT
ATOM		42.667 11.446 4.152 1.00 25.39	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	42.261 11.886 5.491 1.00 28.61	PROT
ATOM		41.463 10.804 6.217 1.00 17.29	PROT
ATOM		40.893 11.224 7.572 1.00 9.05	PROT
ATOM		40.174 12.547 7.435 1.00 17.23	PROT
ATOM	· · · · · · · · · · · · · · · · · · ·	39.946 10.148 8.079 1.00 8.05	PROT
ATOM		43.479 12.234 6.316 1.00 23.36	PROT
ATOM		43.484 13.225 7.037 1.00 10.99	PROT
ATOM		44.503 11.394 6.205 1.00 14.26	PROT
ATOM		45.769 11.595 6.902 1.00 15.33	PROT
ATOM	1822 CB PHE 455	46.761 10.496 6.501 1.00 26.32	PROT
ATOM	1823 CG PHE 455	48.138 10.644 7.108 1.00 43.03	PROT
ATOM		48.305 11.094 8.414 1.00 43.52	PROT
ATOM	1825 CD2 PHE 455	49.270 10.282 6.380 1.00 41.44	PROT
ATOM	1826 CE1 PHE 455	49.576 11.176 8.987 1.00 37.77	PROT
ATOM	1827 CE2 PHE 455	50.536 10.363 6.947 1.00 49.43	PROT
ATOM	1828 CZ PHE 455	50.686 10.811 8.255 1.00 39.99	PROT
ATOM	1829 C PHE 455	46.313 12.956 6.500 1.00 19.37	PROT
ATOM	1830 O PHE 455	46.945 13.646 7.298 1.00 29.31	PROT
ATOM ATOM	1831 N LEU 456 1832 CA LEU 456	46.048 13.345 5.257 1.00 17.16	PROT
ATOM		46.527 14.625 4.750 1.00 20.15	PROT
ATOM	1833 CB LEU 456 1834 CG LEU 456	46.572 14.603 3.218 1.00 35.14 47.593 13.660 2.568 1.00 40.45	PROT
ATOM	1835 CD1 LEU 456		PROT
ATOM	1836 CD2 LEU 456	47.233 13.456 1.116 1.00 44.38 48.990 14.234 2.680 1.00 34.88	PROT
ATOM	1837 C LEU 456	45.680 15.800 5.226 1.00 20.37	PROT PROT
ATOM	1838 O LEU 456	46.207 16.866 5.548 1.00 29.61	PROT
ATOM	1839 N GLU 457	44.367 15.607 5.280 1.00 13.06	PROT
ATOM	1840 CA GLU 457	43.483 16.675 5.713 1.00 14.14	PROT
ATOM	1841 CB GLU 457	42.037 16.256 5.516 1.00 29.57	PROT
ATOM	1842 C GLU 457	43.731 17.058 7.173 1.00 14.95	PROT
ATOM	1843 O GLU 457	43.771 18.237 7.514 1.00 15.98	PROT
ATOM	1844 N VAL 458	43.901 16.051 8.026 1.00 26.34	PROT
ATOM	1845 CA VAL 458	44.143 16.260 9.455 1.00 24.39	PROT
ATOM	1846 CB VAL 458	44.219 14.910 10.208 1.00 20.14	PROT
ATOM	1847 CG1 VAL 458	44.882 15.102 11.554 1.00 22.01	PROT
ATOM	1848 CG2 VAL 458	42.831 14.341 10.400 1.00 28.11	PROT
ATOM	1849 C VAL 458	45.417 17.039 9.778 1.00 21.50	PROT
		11.005 51110 1,00 M1.50	1101

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ATOM	•	0 O	VAL	458	45.36	4 18.0	62 10.4	39 1.00 18.8	B5 PROT
ATOM	1 185	1 N	PHE	459	46.557	7 16.54	16 9.30	08 1.00 16.0	
ATOM	I 185	2 C/	A PHE	459	47.84	0 17.1	74 9.5		
ATOM	I 185	3 CI	3 PHE	459	48.86	2 16.0	72 9.8		
ATOM	[185 ₋	4 CC	3 PHE	459	48.38	9 15.0	55 10.8		
ATOM	[185.	5 CI	O1 PHE	459	47.91	7 13.8			
ATOM	185	6 CI	D2 PHE	459	48.39	0 15.3	39 12.2		
ATOM	185	7 CE	E1 PHE	459	47.44	7 12.8	76 11.3		
ATOM	185	8 CE	2 PHE	459	47.92	2 14.4	02 13.1		
ATOM	1859	9 CZ	PHE	459	47.450	13.17	72 12.7		
ATOM	1860) C	PHE	459	48.381	18.15	2 8.54		
ATOM	186	10	PHE	459	49.601	18.31	1 8.41		
ATOM	1862	2 N	GLU	460	47.480	18.81	6 7.81		
ATOM	1863	CA	GLU	460	47.84	6 19.7			
ATOM	1864	CB	GLU	460	48.930	20.73	32 7.25		
ATOM	1865	CG	GLU	460	48.40				
ATOM	1866	CD	GLU	460	47.29	8 22.6	36 7.3		
ATOM	1867	OE	1 GLU	460	47.44	8 23.8	59 7.1 :	21 1.00 71.9	•
ATOM	1868	OE	2 GLU	460	46.28	0 21.9	93 6.9	98 1.00 72.7	
ATOM	1869	C	GLU	460	48.353	19.03	7 5.53	5 1.00 46.31	
ATOM	1870	0	GLU	460	48.642	17.82	9 5.65	5 1.00 51.79	
ATOM	1871	OT	GLU	460	48.461	19.66	59 4.46	52 1.00 60.93	2 PROT
ATOM	1872		GC1	1	47.011	4.539	15.912	1.00 29.38	LIGA
ATOM	1873		GC1	1	51.292	6.537	13.571	1.00 17.11	LIGA
ATOM	1874		GC1	1	47.393	4.205	14.573	1.00 33.72	LIGA
ATOM	1875		GC1	1	52.119	6.409	12.400	1.00 19.76	LIGA
ATOM	1876		GC1	1	48.689	4.481	14.089	1.00 25.02	LIGA
ATOM	1877		GC1	1	52.344	7.525	11.539	1.00 17.51	LIGA
ATOM	1878		GC1	1	49.684	5.122	14.949	1.00 23.99	LIGA
ATOM	1879		GC1	1	51.722	8.778	11.873	1.00 20.21	LIGA
ATOM	1880		GC1	1	49.283	5.452	16.318	1.00 18.19	LIGA
ATOM			GC1	1	50.906			1.00 15.43	LIGA
ATOM			GC1	1	47.973			1.00 30.64	LIGA
ATOM			GC1	1	50.696			1.00 25.06	LIGA
ATOM	1884		GC1	1	45.700			1.00 28.60	LIGA
ATOM			GC1	1	53.198			1.00 20.30	LIGA
ATOM	1886			1	45.305			1.00 18.51	LIGA
ATOM			GC1	1	52.423			1.00 17.21	LIGA
ATOM			GC1	1	43.816			1.00 21.43	LIGA
ATOM	1889			1	54.514			1.00 24.97	LIGA
ATOM	1890			1	48.994			1.00 33.46	LIGA
ATOM	1891			1	50.243			1.00 27.69	LIGA
ATOM	1892		GC1	1	51.902	9.861		1.00 23.34	LIGA
ATOM	1893		GC1	1	51.026			1.00 22.49	LIGA
ATOM		O3		1				1.00 18.06	LIGA
ATOM	1895	U 4	GCI	1	43.331	5.204	17.065	1.00 28.27	LIGA

END

APPENDIX 8

TRBGC1.PDB

REMARK TR-beta GC-2 Full length numbering REMARK refinement resolution: 100.00 - 2.40 A starting r = 0.2602 free r = 0.2960REMARK final r = 0.2532 free r = 0.2894REMARK sg = P3(1)21 a = 68.9 b = 68.9 c = 131.5 alpha = 90 beta = 90 gamma = 120 REMARK theoretical total number of refl. in resol. range: 14710 (100.0 %) REMARK number of unobserved reflections (no entry or |F| = 0): 336 (2.3 %) REMARK number of reflections rejected: 0 (0.0 %) REMARK total number of reflections used: 14374 (97.7 %) REMARK number of reflections in working set: 13656 (92.8 %) REMARK number of reflections in test set: 718 (4.9 %) REMARK REMARK ALA 199 to ALA 201 from His-tag REMARK REMARK Four cacodylate-modified cysteines (CYA) REMARK Cys294, Cys298, Cys388, Cys434 REMARK cacodylate modeled as single arsenic atom REMARK REMARK side chain of certain residues modeled as ALA due to poor density; REMARK however, residue name reflects true residue for clarity REMARK REMARK amino acid sequence confirmed. REMARK differing from that reported by Weinberger et. al. REMARK in the following codons: REMARK 243 Pro - Arg REMARK 337 lle - Thr REMARK 451 Leu - Phe REMARK as reported by Sakurai et. al. REMARK note also correction of initiation codon. REMARK yielding a polypeptide of 461 amino acids JRNL AUTH A.SAKURAI, A.NAKAI, L.J. DEGROOT JRNL TITL STRUCTURAL ANALYSIS OF HUMAN THYROID HORMONE RECEPTOR JRNL TITL2 BETA GENE JRNL REF MOL.CELL.ENDO. V.71 1990 JRNL AUTH C.WEINBERGER, C.C.THOMPSON, R.LEBO, D.J. GRUOL, R.M. EVANS JRNL TITL THE C-ERB-A GENE ENCODES A THYROID HORMONE RECEPTOR JRNL REF NATURE V.324 6098 1986 ATOM 1 CB ALA 199 36.564 26.104 43.169 1.00 73.87 ATOM 2 C ALA 199 34.723 26.996 44.613 1.00 78.22 ATOM 3 O ALA 199 34.741 28.230 44.568 1.00 81.84 4 N ALA 199 ATOM 34.389 26.744 42.166 1.00 77.76 5 CA ALA 199

35.048 26.165 43.375 1.00 77.98

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ATOM

ATOM	6 N ALA 200	34.428 26.309 45.713 1.00 77.78
ATOM	7 CA ALA 200	34.098 26.961 46.984 1.00 77.03
ATOM	8 CB ALA 200	32.761 27.693 46.865 1.00 79.04
ATOM	9 C ALA 200	34.028 25.897 48.084 1.00 75.79
ATOM	10 O ALA 200	34.877 25.857 48.978 1.00 71.58
ATOM	11 N - ALA 201	33.005 25.050 48.010 1.00 73.70
ATOM	12 CA ALA 201	32.838 23.968 48.972 1.00 70.15
ATOM	13 CB ALA 201	31.468 23.328 48.809 1.00 71.16
ATOM	14 C ALA 201	33.934 22.963 48.642 1.00 67.54
ATOM	15 O ALA 201	34.218 22.044 49.413 1.00 67.14
ATOM	16 N GLU 202	34.540 23.164 47.476 1.00 62.05
ATOM	17 CA GLU 202	35.624 22.325 46.975 1.00 59.45
ATOM	18 CB GLU 202	35.835 22.621 45.482 1.00 55.12
ATOM	19 CG GLU 202	36.820 21.716 44.749 1.00 56.25
ATOM	20 CD GLU 202	36.382 20.260 44.723 1.00 54.99
ATOM	21 OE1 GLU 202	35.216 19.990 44.361 1.00 53.83
ATOM	22 OE2 GLU 202	37.210 19.385 45.050 1.00 59.90
ATOM	23 C GLU 202	36.885 22.674 47.770 1.00 55.96
ATOM	24 O GLU 202	37.472 21.823 48.435 1.00 52.90
ATOM	25 N GLU 203	37.282 23.943 47.698 1.00 54.95
ATOM	26 CA GLU 203	38.464 24.434 48.390 1.00 55.59
ATOM	27 CB GLU 203	38.632 25.924 48.126 1.00 53.21
ATOM	28 C GLU 203	38.415 24.171 49.894 1.00 56.30
ATOM	29 O GLU 203	39.445 23.948 50.526 1.00 58.70
ATOM	30 N LEU 204	37.213 24.193 50.462 1.00 57.14
ATOM	31 CA LEU 204	37.038 23.966 51.893 1.00 56.93
ATOM	32 CB LEU 204	35.658 24.465 52.338 1.00 58.31
ATOM	33 CG LEU 204	35.348 24.508 53.839 1.00 51.69
ATOM	34 CD1 LEU 204	36.314 25.446 54.549 1.00 44.38
ATOM	35 CD2 LEU 204	33.920 24.986 54.039 1.00 52.44
ATOM	36 C LEU 204	37.198 22.489 52.246 1.00 58.20
ATOM	37 O LEU 204	37.831 22.155 53.252 1.00 58.99
ATOM	38 N GLN 205	36.620 21.607 51.431 1.00 58.26
ATOM	39 CA GLN 205	36.736 20.167 51.657 1.00 55.38
ATOM	40 CB GLN 205	35.993 19.377 50.584 1.00 54.52
ATOM	41 CG GLN 205	34.498 19.324 50.741 1.00 53.33
ATOM	42 CD GLN 205	33.854 18.520 49.629 1.00 53.40
ATOM ATOM	43 OE1 GLN 205	33.850 18.939 48.473 1.00 51.68
ATOM	44 NE2 GLN 205 45 C GLN 205	33.325 17.352 49.968 1.00 51.34
ATOM	45 C GLN 205 46 O GLN 205	38.200 19.775 51.608 1.00 55.05
ATOM		38.665 18.964 52.407 1.00 53.63
ATOM	47 N LYS 206 48 CA LYS 206	38.918 20.348 50.648 1.00 53.55 40.337 20.078 50.493 1.00 57.40
ATOM	49 CB LYS 206	40.337 20.078 50.493 1.00 57.40 40.896 20.814 49.269 1.00 58.94
ATOM	50 CG LYS 206	40.300 20.375 47.941 1.00 67.73
ATOM	51 CD LYS 206	40.921 21.141 46.781 1.00 67.73
AT OM	JI CD LIS 200	TU.721 21.141 40./01 1.UU /2.3U

ATOM . 52 CE LYS 206 40.346 20.695 45.445 1.00 75.60 **ATOM** 53 NZ LYS 206 40.945 21.445 44.304 1.00 77.08 **ATOM** 54 C LYS 206 41.053 20.559 51.747 1.00 53.98 **ATOM** 55 O LYS 206 41.905 19.866 52.300 1.00 53.49 **ATOM** 56 N SER 207 40.680 21.757 52.184 1.00 53.61 **ATOM** 57 CA SER 207 41.254 22.386 53.364 1.00 51.49 **ATOM** 58 CB SER 207 40.546 23.715 53.619 1.00 51.01 **ATOM** 59 OG SER 207 41.108 24.383 54.731 1.00 63.00 **ATOM** 60 C SER 207 41.178 21.502 54.616 1.00 49.49 61 O **ATOM** SER 207 42.073 21.538 55.465 1.00 47.44 **ATOM** 62 N ILE 208 40.117 20.707 54.725 1.00 44.39 **ATOM** 63 CA ILE 208 39.938 19.829 55.874 1.00 45.99 **ATOM** 64 CB ILE 208 38.421 19.627 56.174 1.00 44.50 **ATOM** 65 CG2 ILE 208 38.226 18.801 57.445 1.00 49.37 **ATOM** 66 CG1 ILE 208 37.766 20.993 56.385 1.00 42.73 **ATOM** 67 .CD1 ILE 208 36.266 20.941 56.567 1.00 44.13 **ATOM** 68 C ILE 208 40.614 18.477 55.643 1.00 47.80 **ATOM** 69 O ILE 208 40.735 17.666 56.562 1.00 49.81 70 N **ATOM** GLY 209 41.059 18.238 54.412 1.00 51.31 **ATOM** 71 CA GLY 209 41.728 16.983 54.107 1.00 46.85 **ATOM** 72 C GLY 209 40.813 15.896 53.573 1.00 48.31 73 O GLY 209 **ATOM** 41.203 14.730 53.485 1.00 47.75 **ATOM** 74 N HIS 210 39.582 16.274 53.237 1.00 46.79 75 CA HIS 210 **ATOM** 38.622 15.326 52.686 1.00 47.34 **ATOM** 76 CB HIS 210 37.200 15.739 53.068 1.00 49.39 **ATOM** 77 C HIS 210 38.796 15.350 51.162 1.00 45.47 210 **ATOM** 78 O HIS 38.924 16.420 50.566 1.00 41.32 79 N LYS **ATOM** 211 38.829 14.176 50.545 1.00 45.76 **ATOM** 80 CA LYS 211 38.991 14.095 49.090 1.00 43.42 **ATOM** 81 CB LYS 211 39.892 12.910 48.715 1.00 46.72 **ATOM** 82 CG LYS 211 41.210 12.815 49.497 1.00 56.48 **ATOM** 83 CD LYS 211 42.068 14.089 49.486 1.00 60.93 **ATOM** 84 CE LYS 211 42.562 14.496 48.103 1.00 61.95 **ATOM** 85 NZ LYS 211 41.485 15.024 47.218 1.00 69.93 86 C LYS 211 **ATOM** 37.609 13.917 48.473 1.00 35.68 **ATOM** 87 O LYS 211 37.019 12.847 48.557 1.00 33.58 **ATOM** 88 N PRO 37.077 14.972 47.828 1.00 35.64 212 **ATOM** 89 CD PRO 212 37.654 16.304 47.584 1.00 38.60 **ATOM** 90 CA PRO 212 35.748 14.896 47.211 1.00 38.35 91 CB PRO **ATOM** 212 35.537 16.318 46.682 1.00 38.95 92 CG PRO 212 **ATOM** 36.409 17.156 47.604 1.00 42.00 **ATOM** 93 C PRO 212 35.635 13.865 46.096 1.00 38.78 212 36.546 13.714 45.280 1.00 34.64 **ATOM** 94 O PRO **ATOM** 95 N GLU 213 34.517 13.153 46.077 1.00 40.31 **ATOM** 96 CA GLU 213 34.256 12.160 45.049 1.00 43.87 **ATOM** 97 CB GLU 213 33.722 10.873 45.684 1.00 45.16

ATOM 98 CG GLU 213 34.616 10.344 46.800 1.00 47.60 ATOM · 99 CD GLU 213 34.404 8.870 47.088 1.00 50.68 100 OE1 GLU **ATOM** 213 33.240 8.416 47.072 1.00 59.18 **ATOM** 101 OE2 GLU 213 35.402 8.167 47.353 1.00 49.06 102 C GLU 213 **ATOM** 33.234 12.796 44.083 1.00 45.96 **ATOM** 103 O. GLU 213 32.703 13.876 44.368 1.00 43.13 **ATOM** 104 N PRO 214 32.953 12.154 42.933 1.00 46.52 **ATOM** 105 CD PRO 214 33.459 10.884 42.391 1.00 46.44 106 CA PRO **ATOM** 214 31.995 12.737 41.982 1.00 47.52 **ATOM** 107 CB PRO 214 32.040 11.750 40.813 1.00 45.40 **ATOM** 108 CG PRO 214 33.445 11.181 40.913 1.00 49.89 **ATOM** 109 C PRO 214 30.564 12.969 42.465 1.00 45.70 **ATOM** 110 O PRO 29.972 12.112 43.121 1.00 44.49 214 THR **ATOM** 111 N 215 30.013 14.136 42.129 1.00 45.24 **ATOM** 112 CA THR 215 28.629 14.447 42.483 1.00 49.36 **ATOM** 113 CB THR 215 28.312 15.949 42.330 1.00 44.86 **ATOM** 114 OG1 THR 215 28.253 16.285 40.942 1.00 52.26 115 CG2 THR 215 **ATOM** 29.387 16.793 42.992 1.00 39.43 **ATOM** 116 C THR 215 27.791 13.673 41.464 1.00 52.51 **ATOM** 117 O THR 215 28.326 13.192 40.465 1.00 53.48 **ATOM** 118 N ASP 216 26.491 13.543 41.712 1.00 58.81 **ATOM** 119 CA ASP 25.603 12.810 40.805 1.00 61.51 216 **ATOM** 120 CB ASP 216 24.150 12.941 41.270 1.00 70.57 **ATOM** 121 CG ASP 216 23.902 12.257 42.595 1.00 78.07 **ATOM** 122 OD1 ASP 216 24.042 11.018 42.660 1.00 82.31 **ATOM** 123 OD2 ASP 216 23.572 12.962 43.571 1.00 86.55 **ATOM** 124 C ASP 216 25.706 13.277 39.356 1.00 58.42 **ATOM** 125 O ASP 216 25.695 12.464 38.429 1.00 56.85 **ATOM** 126 N GLU 217 25.798 14.587 39.167 1.00 54.92 **ATOM** 127 CA GLU 217 25.905 15.156 37.833 1.00 53.37 **ATOM** 128 CB GLU 217 25.861 16.682 37.906 1.00 51.02 **ATOM** 129 C GLU 217 27.211 14.692 37.195 1.00 53.55 **ATOM** 130 O GLU 217 27.239 14.301 36.027 1.00 54.33 **ATOM** 131 N GLU 218 28.290 14.726 37.975 1.00 49.20 **ATOM** 132 CA GLU 218 29.593 14.310 37.486 1.00 45.94 **ATOM** 133 CB GLU 218 30.674 14.601 38.530 1.00 43.43 **ATOM** 134 CG GLU 218 30.787 16.069 38.878 1.00 40.86 **ATOM** 135 CD GLU 218 31.930 16.347 39.826 1.00 39.88 **ATOM** 136 OE1 GLU 218 32.000 15.667 40.875 1.00 37.61 **ATOM** 137 OE2 GLU 218 32.748 17.250 39.529 1.00 34.01 **ATOM** 138 C GLU 218 29.624 12.838 37.101 1.00 44.71 **ATOM** 139 O GLU 218 30.275 12.471 36.130 1.00 45.31 **ATOM** 140 N TRP 219 28.935 11.991 37.863 1.00 44.02 ATOM 141 CA TRP 219 28.892 10.572 37.539 1.00 46.97 **ATOM** 142 CB TRP 219 28.183 9.762 38.630 1.00 48.42 **ATOM** 143 CG TRP 219 29.034 9.473 39.823 1.00 54.61

ATOM 144 CD2 TRP 219 30.167 8.572 39.879 1.00 55.24 145 CE2 TRP ATOM 219 30.659 8.610 41.201 1.00 53.67 **ATOM** 146 CE3 TRP 219 30.795 7.745 38.938 1.00 54.55 **ATOM** 147 CD1 TRP 219 28.902 10.000 41.074 1.00 55.75 **ATOM** 148 NE1 TRP 219 29.868 9.491 41.912 1.00 54.43 **ATOM** 149 CZ2 TRP 219 31.771 7.846 41.622 1.00 52.54 **ATOM** 150 CZ3 TRP 219 31.912 6.975 39.353 1.00 55.17 **ATOM** 151 CH2 TRP 219 32.380 7.038 40.690 1.00 55.59 **ATOM** 152 C TRP 219 28.167 10.356 36.216 1.00 47.32 **ATOM** 153 O TRP 219 28.433 9.384 35.503 1.00 43.56 **ATOM** 154 N GLU 220 27.247 11.259 35.898 1.00 49.91 **ATOM** 155 CA GLU 220 26.497 11.155 34.655 1.00 53.57 **ATOM** 156 CB GLU 220 25.274 12.075 34.694 1.00 58.18 **ATOM** 157 CG GLU 220 24.323 11.876 33.526 1.00 73.13 **ATOM** 158 CD GLU 220 23.082 12.742 33.630 1.00 80.06 **ATOM** 159 OE1 GLU 220 22.348 12.619 34.636 1.00 82.12 **ATOM** 160 OE2 GLU 220 22.839 13.545 32.701 1.00 82.78 ATOM 161 C GLU 220 27.419 11.534 33.497 1.00 50.51 27.399 10.899 32.443 1.00 49.94 ATOM 162 O GLU 220 **ATOM** 163 N LEU 221 28.232 12.567 33.711 1.00 43.71 **ATOM** 164 CA LEU 221 29.187 13.019 32.702 1.00 42.81 **ATOM** 165 CB LEU 221 29.868 14.317 33.155 1.00 39.21 **ATOM** 166 CG LEU 221 30.945 14.949 32.261 1.00 36.34 **ATOM** 167 CD1 LEU 221 30.339 15.351 30.922 1.00 36.93 **ATOM** 168 CD2 LEU 221 31.535 16.164 32.949 1.00 24.18 **ATOM** 169 C LEU 221 30.234 11.928 32.505 1.00 43.46 **ATOM** 170 O LEU 221 30.618 11.621 31.375 1.00 45.25 ATOM 171 N ILE 222 30.683 11.342 33.614 1.00 39.09 **ATOM** 172 CA ILE 222 31.677 10.273 33.586 1.00 35.47 **ATOM** 173 CB ILE 222 32.031 9.811 35.037 1.00 33.74 **ATOM** 174 CG2 ILE 222 32.822 8.505 35.018 1.00 28.86 **ATOM** 175 CG1 ILE 222 32.813 10.918 35.745 1.00 33.33 **ATOM** 176 CD1 ILE 222 33.111 10.646 37.199 1.00 34.85 **ATOM** 177 C ILE 222 31.139 9.098 32.781 1.00 34.26 **ATOM** 178 O ILE 222 31.877 8.427 32.070 1.00 31.90 **ATOM** 179 N LYS 223 29.840 8.860 32.908 1.00 39.49 **ATOM** 180 CA LYS 223 29.168 7.775 32.210 1.00 44.43 **ATOM** 181 CB LYS 223 27.696 7.733 32.635 1.00 50.81 **ATOM** 182 .CG LYS 223 26.845 6.693 31.929 1.00 62.51 **ATOM** 183 CD LYS 223 25.379 6.856 32.313 1.00 72.22 **ATOM** 184 CE LYS 223 24.487 5.855 31.591 1.00 74.55 **ATOM** 185 NZ LYS 223 23.045 6.057 31.925 1.00 75.78 **ATOM** 186 C LYS 223 29.266 7.983 30.691 1.00 42.81 **ATOM** 187 O LYS 223 29.640 7.078 29.946 1.00 40.36 **ATOM** THR 224 28.924 188 N 9.194 30.257 1.00 39.89 **ATOM** 189 CA THR 224 28.948 9.566 28.850 1.00 39.93

ATOM 190 CB THR 224 28.466 11.021 28.680 1.00 40.57 **ATOM** 191 OG1 THR 224 27.135 11.134 29.197 1.00 39.27 **ATOM** 192 CG2 THR 224 28.480 11.437 27.214 1.00 38.11 **ATOM** 193 C THR 224 30.333 9.433 28.234 1.00 39.96 **ATOM** 194 O THR 224 30.515 8.714 27.248 1.00 36.67 **ATOM** 195 N- VAL 225 31.303 10.123 28.833 1.00 38.02 **ATOM** 196 CA VAL 225 32.680 10.117 28.355 1.00 38.12 **ATOM** 197 CB VAL 225 33.565 11.014 29.243 1.00 38.19 **ATOM** 198 CG1 VAL 225 34.960 11.162 28.632 1.00 36.77 **ATOM** 199 CG2 VAL 225 32.910 12.361 29.406 1.00 41.76 **ATOM** 200 C VAL 225 33.291 8.724 28.302 1.00 37.52 **ATOM** 201 O VAL 225 34.022 8.395 27.364 1.00 36.77 **ATOM** 202 N THR 226 33.002 7.904 29.310 1.00 34.02 **ATOM** 203 CA THR 226 33.542 6.552 29.350 1.00 34.67 ATOM 204 CB THR 226 33.237 5.857 30.707 1.00 30.56 **ATOM** 205 OG1 THR 226 33.858 6.598 31.768 1.00 32.20 **ATOM** 206 CG2 THR 226 33.775 4.437 30.722 1.00 20.99 **ATOM** 207 C THR 226 32.960 5.722 28.211 1.00 36.41 **ATOM** 208 O THR 226 33.698 5.075 27.472 1.00 39.64 **ATOM** 209 N GLU 227 31.636 5.758 28.073 1.00 39.20 ATOM 210 CA GLU 227 30.935 5.020 27.027 1.00 36.93 ATOM 211 CB GLU 227 29.434 5.296 27.111 1.00 38.06 212 C GLU 227 **ATOM** 31.466 5.409 25.651 1.00 37.69 **ATOM** 213 O GLU 227 31.713 4.544 24.805 1.00 40.94 **ATOM** 214 N ALA 228 31.641 6.709 25.439 1.00 32.86 **ATOM** 215 CA ALA 228 32.156 7.236 24.177 1.00 32.48 **ATOM** 216 CB ALA 228 32.285 8.746 24.256 1.00 28.25 **ATOM** 217 C ALA 228 33.508 6.612 23.861 1.00 36.12 **ATOM** 218 O ALA 228 33.736 6.135 22.747 1.00 37.86 **ATOM** 219 N HIS 229 34.404 6.611 24.843 1.00 33.58 **ATOM** 220 CA HIS 229 35.724 6.029 24.669 1.00 32.97 **ATOM** 221 CB HIS 229 36.579 6.263 25.921 1.00 33.69 **ATOM** 222 CG HIS 229 37.857 5.489 25.934 1.00 28.39 **ATOM** 223 CD2 HIS 229 38.338 4.576 26.811 1.00 28.83 **ATOM** 224 ND1 HIS 229 38.804 5.593 24,937 1.00 30.47 **ATOM** 225 CE1 HIS 229 39.812 4.779 25.193 1.00 26.95 **ATOM** 226 NE2 HIS 229 39.556 4.147 26.332 1.00 31.27 **ATOM** 227 C HIS 229 35.653 4.536 24.371 1.00 38.40 **ATOM** 228 O HIS 229 36.227 4.071 23.383 1.00 41.49 **ATOM** 229 N VAL 230 34.951 3.786 25.216 1.00 38.55 ATOM 34.823 2.339 25.049 1.00 40.40 230 CA VAL 230 **ATOM** 231 CB VAL 230 33.964 1.726 26.196 1.00 44.68 **ATOM** 232 CG1 VAL 230 33.865 0.208 26.041 1.00 39.39 **ATOM** 233 CG2 VAL 230 34.576 2.075 27.540 1.00 42.18 **ATOM** 234 C VAL 230 34.219 1.934 23.700 1.00 44.28 **ATOM** 235 O VAL 230 34.640 0.948 23.092 1.00 45.94

ATOM 236 N ALA 231 33.236 2.698 23.230 1.00 45.59 **ATOM** 237 CA ALA 231 32.580 2.403 21.961 1.00 47.84 **ATOM** 238 CB ALA 31.297 3.227 21.832 1.00 45.08 231 **ATOM** 239 C ALA 231 33.487 2.666 20.761 1.00 48.04 **ATOM** 240 O ALA 33.364 231 2.012 19.727 1.00 49.95 **ATOM** 241 N- THR 232 34.403 3.619 20.907 1.00 47.26 **ATOM** 242 CA THR 232 35.312 3.973 19.824 1.00 43.64 **ATOM** 243 CB THR 232 35.379 5.502 19.629 1.00 41.93 **ATOM** 244 OG1 THR 232 35.945 6.117 20.797 1.00 39.10 **ATOM** 245 CG2 THR 232 33.985 6.065 19.382 1.00 29.80 **ATOM** 246 C THR 232 36.720 3.458 20.046 1.00 43.97 **ATOM** 247 O THR 232 37.629 3.791 19.292 1.00 40.55 248 N ASN **ATOM** 233 36.905 2.648 21.081 1.00 48.62 **ATOM** 249 CA ASN 233 38.218 2.101 21.368 1.00 58.62 **ATOM** 250 CB ASN 233 38.473 2.092 22.876 1.00 62.44 **ATOM** 251 CG ASN 233 39.909 1.765 23.223 1.00 68.35 **ATOM** 252 OD1 ASN 233 40.843 2.401 22.724 1.00 65.50 **ATOM** 253 ND2 ASN 233 40.098 0.776 24.090 1.00 74.29 **ATOM** 254 C ASN 233 38.282 0.690 20.802 1.00 65.06 **ATOM** 255 O ASN 233 37.748 -0.257 21.382 1.00 69.47 **ATOM** 256 N ALA 234 38.934 0.577 19.645 1.00 68.80 **ATOM** 257 CA ALA 234 39.098 -0.672 18.909 1.00 70.98 **ATOM** 258 CB ALA 234 40.215 -0.508 17.886 1.00 71.43 **ATOM** 259 C ALA 234 39.353 -1.919 19.753 1.00 73.83 **ATOM** 260 O ALA 234 40.193 -1.911 20.652 1.00 74.33 **ATOM** 261 N GLN 235 38.615 -2.983 19.434 1.00 75.07 **ATOM 262 CA GLN** 235 38.720 -4.281 20.103 1.00 76.32 **ATOM** 263 CB GLN 235 40.130 -4.856 19.912 1.00 76.98 **ATOM** 264 CG GLN 235 40.429 -5.417 18.516 1.00 77.07 **ATOM** 265 CD GLN 235 40.142 -4.444 17.377 1.00 80.85 **ATOM** 235 266 OE1 GLN 38.985 -4.144 17.072 1.00 82.01 **ATOM** 267 NE2 GLN 235 41.201 -3.949 16.742 1.00 78.80 **ATOM** 268 C GLN 235 38.351 -4.293 21.586 1.00 77.15 **ATOM** 269 O GLN 235 38.217 -5.361 22.190 1.00 76.06 **ATOM** 270 N GLY 236 38.188 -3.103 22,161 1.00 77.46 **ATOM** 271 CA GLY 236 37.818 -2.974 23.562 1.00 78.37 **ATOM** 272 C GLY 236 38.620 -3.783 24.566 1.00 79.43 **ATOM** 273 O GLY 236 39.826 -3.575 24.736 1.00 79.47 SER 237 **ATOM** 274 N 37.937 -4.711 25.234 1.00 77.98 **ATOM** 275 CA SER 237 38.544 -5.561 26.253 1.00 76.49 **ATOM** 237 276 CB SER 37.475 -6.462 26.874 1.00 76.46 **ATOM** 277 C SER 237 39.712 -6.412 25.765 1.00 75.35 **ATOM** 278 O SER 237 40.858 -6.181 26.152 1.00 75.47 **ATOM** 279 N HIS 238 39.421 -7.397 24.922 1.00 75.56 280 CA HIS 238 **ATOM** 40.451 -8.294 24.409 1.00 75.46 **ATOM** 281 CB HIS 238 39.837 -9.654 24.076 1.00 75.85

ATOM 282 C HIS 238 41.185 -7.751 23.191 1.00 74.10 **ATOM** 283 O HIS 238 40.610 -7.638 22.109 1.00 75.34 284 N **ATOM** TRP 239 42.459 -7.417 23.381 1.00 73.39 **ATOM** 285 CA TRP 239 43.300 -6.907 22.302 1.00 74.02 **ATOM** 286 CB TRP 239 43.556 -5.402 22.460 1.00 81.77 **ATOM** 287 CG TRP 239 44.190 -5.023 23.761 1.00 89.67 **ATOM** 288 CD2 TRP 239 45.597 -4.797 24.008 1.00 93.19 **ATOM** 289 CE2 TRP 239 45.744 -4.527 25.384 1.00 95.46 **ATOM** 290 CE3 TRP 239 46.732 -4.793 23.186 1.00 95.35 **ATOM** 291 CD1 TRP 239 43.566 -4.888 24.972 1.00 94.16 **ATOM** 292 NE1 TRP 239 44.483 -4.591 25.954 1.00 97.48 **ATOM** 293 CZ2 TRP 239 46.993 -4.262 25.981 1.00 96.23 294 CZ3 TRP **ATOM** 239 47.992 -4.528 23.778 1.00 96.75 **ATOM** 295 CH2 TRP 239 48.101 -4.262 25.164 1.00 97.32 **ATOM** 296 C TRP 239 44.633 -7.649 22.283 1.00 70.77 **ATOM** 297 O TRP 239 45.339 -7.644 21.274 1.00 71.70 **ATOM** 298 N LYS 240 44.978 -8.276 23.405 1.00 67.10 **ATOM** 299 CA LYS 240 46.219 -9.040 23.519 1.00 65.63 **ATOM** 300 CB LYS 240 46.387 -9.569 24.946 1.00 66.65 **ATOM** 301 CG LYS 240 46.379 -8.504 26.030 1.00 69.83 **ATOM** 302 CD LYS 240 47.664 -7.691 26.069 1.00 71.49 **ATOM** 303 CE LYS 240 48.839 -8.515 26.573 1.00 71.31 **ATOM** 304 NZ LYS 240 50.071 -7.684 26.691 1.00 72.23 **ATOM** 305 C LYS 240 46.143 -10.222 22.555 1.00 66.19 **ATOM** 306 O LYS 240 47.075 -10.493 21.797 1.00 65.20 **ATOM** 307 N ASN 241 45.010 -10.923 22.598 1.00 66.69 **ATOM 308 CA ASN** 241 44.773 -12.089 21.750 1.00 67.53 **ATOM** 309 CB ASN 241 43.503 -12.813 22.213 1.00 67.98 310 CG ASN **ATOM** 43.504 -13.096 23.704 1.00 70.19 241 **ATOM** 311 OD1 ASN 241 44.410 -13.744 24.227 1.00 71.37 **ATOM** 312 ND2 ASN 241 42.483 -12.605 24.400 1.00 71.48 **ATOM** 313 C ASN 241 44.621 -11.681 20.286 1.00 66.62 **ATOM** 314 O ASN 241 44.882 -12.475 19.382 1.00 64.76 **ATOM** 315 N LYS 242 44.196 -10.436 20.070 1.00 66.86 **ATOM** 316 CA LYS 242 43.989 -9.882 18.732 1.00 67.46 **ATOM** 317 CB LYS 42.982 -8.731 18.799 1.00 67.93 242 **ATOM** 318 CG LYS 242 41.601 -9.138 19.279 1.00 71.52 **ATOM** 319 CD LYS 242 40.876 -9.986 18.246 1.00 74.32 **ATOM** 320 CE LYS 242 40.449 -9.160 17.043 1.00 74.41 **ATOM** 321 NZ LYS 242 39.455 -8.120 17.436 1.00 74.44 **ATOM** 322 C LYS 242 45.281 -9.367 18.097 1.00 66.28 **ATOM** 323 O LYS 242 45.414 -9.334 16.874 1.00 67.61 **ATOM** 324 N ARG 243 46.225 -8.961 18.938 1.00 64.19 **ATOM** 325 CA ARG 243 47.497 -8.422 18.478 1.00 62.43 **ATOM** 326 CB ARG 243 48.376 -8.070 19.685 1.00 60.12 **ATOM** 327 C ARG 243 48.261 -9.348 17.538 1.00 62.97

ATOM 328 O ARG 48.585 -10.484 17.891 1.00 63.96 243 **ATOM** 329 N LYS 244 48.531 -8.853 16.334 1.00 62.41 **ATOM** 330 CA LYS 244 49.303 -9.593 15.339 1.00 61.57 **ATOM** 331 CB LYS 244 48.601 -9.607 13.972 1.00 63.68 332 CG LYS **ATOM** 244 47.210 -10.231 13.970 1.00 71.29 **ATOM** 333 CD LYS 244 46.666 -10.441 12.549 1.00 73.83 **ATOM** 334 CE LYS 244 46.505 -9.139 11.767 1.00 74.71 **ATOM** 335 NZ LYS 244 45.542 -8.199 12.407 1.00 73.32 **ATOM** 336 C LYS 244 50.613 -8.824 15.223 1.00 59.30 **ATOM** 337 O LYS 244 50.637 -7.716 14.686 1.00 56.34 **ATOM** 338 N PHE 245 51.690 -9.405 15.744 1.00 57.06 **ATOM** 339 CA PHE 245 52.996 -8.757 15.704 1.00 59.01 **ATOM** 340 CB PHE 245 54.034 -9.588 16.467 1.00 59.62 **ATOM** 341 CG PHE 245 53.704 -9.783 17.934 1.00 66.60 **ATOM** 342 CD1 PHE 245 52.656 -10.626 18.329 1.00 67.17 **ATOM** 343 CD2 PHE 245 54.427 -9.096 18.918 1.00 69.25 **ATOM** 344 CE1 PHE 245 52.320 -10.789 19.699 1.00 69.92 **ATOM** 345 CE2 PHE 245 54.111 -9.240 20.294 1.00 70.50 346 CZ PHE ATOM 53.051 -10.091 20.686 1.00 70.89 245 **ATOM** 347 C PHE 245 53.463 -8.537 14.272 1.00 60.68 **ATOM** 348 O PHE 245 53.433 -9.455 13.447 1.00 62.37 **ATOM** 349 N LEU 246 53.880 -7.311 13.976 1.00 60.10 **ATOM** 350 CA LEU 246 54.359 -6.968 12.642 1.00 59.44 **ATOM** 351 CB LEU 246 54.654 -5.464 12.560 1.00 57.43 **ATOM** 352 CG LEU 246 54.937 -4.851 11.183 1.00 54.41 **ATOM** 353 CD1 LEU 246 53.681 -4.931 10.320 1.00 52.43 **ATOM** 354 CD2 LEU 246 55.358 -3.398 11.343 1.00 51.69 **ATOM** 55.638 -7.772 12.425 1.00 62.05 355 C LEU 246 **ATOM** 56.447 -7.923 13.346 1.00 59.85 356 O LEU 246 **ATOM** 357 N PRO 247 55.836 -8.312 11.203 1.00 63.33 **ATOM** 358 CD PRO 247 54.990 -8.230 10.001 1.00 64.44 **ATOM** 359 CA PRO 247 57.036 -9.102 10.910 1.00 63.56 **ATOM** 360 CB PRO 247 56.917 -9.327 9.404 1.00 64.42 **ATOM** 361 CG PRO 247 55.413 -9.481 9.251 1.00 64.90 **ATOM** 362 C PRO 247 58.342 -8.431 11.325 1.00 61.94 **ATOM** 363 O PRO 58.581 -7.256 11.053 1.00 61.60 247 **ATOM** 364 N ALA 248 59.180 -9.219 11.990 1.00 61.33 **ATOM** 365 CA ALA 248 60.468 -8.785 12.511 1.00 63.50 **ATOM** 366 CB ALA 248 61.151 -9.991 13.174 1.00 66.94 **ATOM** 370 C ALA 248 61.412 -8.140 11.489 1.00 64.19 **ATOM** 371 O ALA 248 62.449 -7.593 11.867 1.00 65.56 **ATOM** 372 N ASP 249 61.055 -8.188 10.207 1.00 64.36 **373 CA ASP ATOM** 249 61.900 -7.610 9.163 1.00 63.33 **ATOM** 374 CB ASP 249 62.104 -8.618 8.026 1.00 62.97 **ATOM** 375 CG ASP 249 60.798 -9.051 7.395 1.00 64.63 **ATOM** 376 OD1 ASP 249 60.037 -9.803 8.043 1.00 64.84

ATOM 377 OD2 ASP 249 60.526 -8.626 6.253 1.00 66.52 **ATOM** 378 C ASP 249 61.388 -6.293 8.572 1.00 64.31 **ATOM** 379 O **ASP** 249 62.112 -5.624 7.830 1.00 64.73 **ATOM** 380 N ILE 250 60.148 -5.927 8.885 1.00 63.09 **ATOM** 381 CA ILE 250 59.577 -4.676 8.385 1.00 64.39 **ATOM** 382 CB ILE 250 58.035 -4.741 8.349 1.00 65.79 ATOM 383 CG2 ILE 250 57.463 -3.408 7.861 1.00 64.78 **ATOM** 384 CG1 ILE 250 57.594 -5.893 7.439 1.00 65.28 **ATOM** 385 CD1 ILE 250 56.094 -6.103 7.362 1.00 65.08 386 C ILE 250 **ATOM** 60.015 -3.534 9.299 1.00 65.21 **ATOM** 387 O ILE 250 60.002 -3.676 10.524 1.00 64.05 **ATOM** 388 N GLY 251 60.401 -2.405 8.700 1.00 65.48 **ATOM** 389 CA GLY 251 60.864 -1.263 9.472 1.00 67.32 **ATOM** 390 C GLY 251 62.069 -1.711 10.271 1.00 68.52 **ATOM** 391 O GLY 251 62.099 -1.610 11.497 1.00 65.49 **ATOM** 392 N GLN 252 63.080 -2.194 9.555 1.00 72.26 **ATOM** 393 CA GLN 252 64.277 -2.726 10.176 1.00 74.10 **ATOM** 394 CB GLN 252 64.598 -4.068 9.515 1.00 75.82 **ATOM** 395 CG GLN 252 65.518 -4.974 10.302 1.00 77.81 **ATOM** 396 CD GLN 252 65.686 -6.319 9.630 1.00 79.38 **ATOM** 397 OE1 GLN 252 66.087 -6.397 8.468 1.00 80.55 **ATOM** 252 398 NE2 GLN 65.384 -7.391 10.357 1.00 78.12 **ATOM** 399 C GLN 252 65.496 -1.817 10.138 1.00 77.17 **ATOM** 400 O GLN 252 65.553 -0.826 9.399 1.00 76.50 **ATOM** 401 N ALA 253 66.470 -2.187 10.966 1.00 80.78 **ATOM** 402 CA ALA 253 67.729 -1.475 11.104 1.00 83.70 **ATOM** 403 CB ALA 253 68.402 -1.903 12.401 1.00 83.23 **ATOM** 404 C ALA 253 68.639 -1.774 9.913 1.00 85.59 **ATOM** 405 O ALA 253 68.294 -2.673 9.117 1.00 85.69 **ATOM** 406 OXT ALA 253 69.694 -1.115 9.802 1.00 88.37 **ATOM** 429 CB LYS 263 65.708 7.766 4.514 1.00 63.50 **ATOM** 430 C LYS 263 64.141 6.903 6.272 1.00 63.41 **ATOM** 431 O LYS 263 64.442 5.776 6.673 1.00 61.93 432 N LYS **ATOM** 263 66.368 7.841 6.894 1.00 61.71 **ATOM** 433 CA LYS 263 65.218 7.942 5.950 1.00 64.36 **ATOM** 434 N VAL 264 62.886 7.305 6.090 1.00 61.15 **ATOM** 435 CA VAL 264 61.724 6.462 6.351 1.00 59.46 **ATOM** 436 CB VAL 264 60.429 7.221 5.962 1.00 59.03 **ATOM** 437 CG1 VAL 264 59.200 6.421 6.363 1.00 53.79 438 CG2 VAL 264 **ATOM** 60.422 8.593 6.623 1.00 55.32 **ATOM** 439 C VAL 264 61.790 5.129 5.595 1.00 60.96 62.071 5.098 4.395 1.00 62.13 **ATOM** 440 O VAL 264 **ATOM** 441 N ASP 265 61.522 4.034 6.304 1.00 62.59 **ATOM** 442 CA ASP 265 61.562 2.693 5.727 1.00 64.95 **ATOM** 443 CB ASP 61.322 1.644 6.810 1.00 64.32 265 **ATOM** 444 CG ASP 265 61.415 0.232 6.277 1.00 67.70

ATOM 445 OD1 ASP 265 62.514 -0.158 5.831 1.00 72.59 **ATOM** 446 OD2 ASP 265 60.393 -0.486 6.289 1.00 68.84 **ATOM** 447 C **ASP** 265 60.560 2.470 4.591 1.00 65.64 **ATOM** 448 O **ASP** 265 60.789 1.637 3.717 1.00 68.81 ATOM 449 N LEU 266 59.456 3.211 4.624 1.00 65.12 **ATOM** 450 CA LEU 266 58.394 3.615 1.00 63.40 3.138 **ATOM** 451 CB LEU 266 58.963 3.333 2.202 1.00 67.34 **ATOM** 452 CG LEU 266 59.665 4.662 1.894 1.00 69.35 ATOM 453 CD1 LEU 266 60.193 4.627 0.469 1.00 68.24 **ATOM** 454 CD2 LEU 266 58.705 5.831 2.075 1.00 70.47 **ATOM** 455 C LEU 266 57.562 1.854 3.658 1.00 59.67 **ATOM** 456 O LEU 266 56.342 1.903 3.486 1.00 53.35 **ATOM** 457 N GLU 267 58.205 0.713 3.872 1.00 58.01 **ATOM** 57.454 -0.535 3.945 1.00 58.34 458 CA GLU 267 **ATOM** 459 CB GLU 267 58.387 -1.750 3.921 1.00 59.21 **ATOM** 460 CG GLU 267 57.640 -3.072 4.053 1.00 62.89 **ATOM** 461 CD GLU 267 58.548 -4.285 3.979 1.00 67.66 **ATOM** 462 OE1 GLU 267 59.513 -4.371 4.771 1.00 69.95 **ATOM** 463 OE2 GLU 267 58.285 -5.162 3.129 1.00 69.40 **ATOM** 464 C GLU 267 56.666 -0.515 5.243 1.00 57.67 **ATOM** 55.488 -0.877 465 O **GLU** 267 5.276 1.00 58.34 **ATOM** 466 N ALA 268 57.327 -0.077 6.317 1.00 53.43 **ATOM** 467 CA ALA 268 56.701 0.013 7.629 1.00 49.00 **ATOM** 468 CB ALA 268 57.766 0.244 8.695 1.00 45.72 **ATOM** 469 C ALA 268 55.701 1.166 7.611 1.00 45.76 **ATOM** 470 O ALA 268 54.598 1.057 8.144 1.00 41.50 **ATOM** 471 N PHE 269 56.106 2.267 6.983 1.00 41.43 472 CA PHE **ATOM** 269 55.277 3.457 6.855 1.00 43.96 **ATOM** 473 CB PHE 269 56.016 4.511 6.022 1.00 40.10 **ATOM** 474 CG PHE 269 55.264 5.818 5.859 1.00 40.44 **ATOM** 475 CD1 PHE 269 55.102 6.690 6.949 1.00 38.98 **ATOM** 476 CD2 PHE 269 54.706 6.170 4.626 1.00 37.15 **ATOM** 477 CE1 PHE 269 54.401 7.920 6.807 1.00 32.12 **ATOM** 478 CE2 PHE 269 53.999 7.389 4.457 1.00 38.41 **ATOM** 479 CZ PHE 269 53.843 8.269 5.554 1.00 40.55 **ATOM** 480 C PHE 269 53.976 6.151 1.00 49.76 3.081 **ATOM** 481 O PHE 269 52.903 3.622 6.443 1.00 52.15 **ATOM** 482 N SER 270 54.089 2.140 5.217 1.00 53.15 **ATOM** 483 CA SER 270 52.957 1.669 4.432 1.00 52.29 **ATOM** 484 CB SER 270 53.456 0.703 3.349 1.00 51.85 **ATOM** 485 OG SER 270 52.400 0.297 2.499 1.00 53.42 **ATOM** 486 C SER 270 51.901 0.992 5.303 1.00 49.38 **ATOM** 487 O SER 270 50.713 1.284 5.185 1.00 48.74 **ATOM** 488 N HIS 271 52.335 0.085 6.173 1.00 50.15 **ATOM** 489 CA HIS 271 51.410 -0.614 7.061 1.00 51.67 **ATOM** 490 CB HIS 271 52.150 -1.682 7.878 1.00 58.52

(Sept.)

ATOM 491 CG HIS 52.697 -2.808 271 7.059 1.00 68.97 **ATOM** 492 CD2 HIS 271 7.063 1.00 70.88 52.425 -4.131 **ATOM** 493 ND1 HIS 271 53.660 -2.621 6.080 1.00 71.98 **ATOM** 494 CE1 HIS 5.528 1.00 73.91 271 53.951 -3.782 **ATOM 495 NE2 HIS** 271 53.214 -4.720 6.104 1.00 73.59 **ATOM** 496 C - HIS 271 50.711 0.365 8.008 1.00 48.33 **ATOM** 497 O HIS 271 49.507 0.260 8.240 1.00 48.39 **ATOM** 498 N PHE 272 51.472 1.321 8.537 1.00 41.34 **ATOM** 499 CA PHE 272 50.946 2.316 9.462 1.00 39.44 **ATOM** 500 CB PHE 272 52.076 3.215 9.976 1.00 36.67 **ATOM** 501 CG PHE 272 2.475 10.749 1.00 33.39 53.167 502 CD1 PHE **ATOM** 272 3.065 10.915 1.00 33.14 54.421 **ATOM** 503 CD2 PHE 272 52.934 1.216 11.311 1.00 38.28 504 CE1 PHE 272 **ATOM** 55.454 2.418 11.633 1.00 38.26 **ATOM** 505 CE2 PHE 272 53.961 0.538 12.047 1.00 43.28 506 CZ PHE **ATOM** 272 55.225 1.146 12.207 1.00 39.74 **ATOM** 507 C PHE 272 49.857 3.183 8.822 1.00 40.75 **ATOM** 508 O PHE 272 48.784 3.361 9.394 1.00 35.51 **ATOM** 509 N THR 273 50.136 3.714 7.635 1.00 41.64 **ATOM** 510 CA THR 273 49.170 4.561 6.938 1.00 45.97 **ATOM** 511 CB THR 273 49.813 5.249 5.711 1.00 51.52 **ATOM** 512 OG1 THR 273 50.339 4.257 4.815 1.00 45.74 **ATOM** 513 CG2 THR 273 50.936 6.179 6.158 1.00 49.73 **ATOM** 514 C THR 273 47.941 3.772 6.481 1.00 46.23 **ATOM** 515 O THR 273 46.879 4.344 6.233 1.00 41.21 **ATOM** 516 N LYS 274 48.090 2.455 6.380 1.00 46.21 46.984 **ATOM** 517 CA LYS 274 1.608 5.955 1.00 54.53 47.482 0.180 5.708 1.00 54.36 **ATOM** 518 CB LYS 274 **ATOM** 519 C LYS 274 45.878 1.595 7.006 1.00 56.88 **ATOM** 520 O LYS 274 44.695 1.486 6.675 1.00 57.98 **ATOM** 521 N ILE 275 46.267 1.718 8.268 1.00 56.48 **ATOM** 522 CA ILE 275 45.312 1.695 9.368 1.00 52.64 **ATOM** 523 CB ILE 275 45.710 0.611 10.391 1.00 49.15 **ATOM** 524 CG2 ILE 275 45.719 -0.758 9.701 1.00 47.42 525 CG1 ILE **ATOM** 275 47.101 0.921 10:971 1.00 45.31 **ATOM** 526 CD1 ILE 275 47.565 -0.050 12.053 1.00 37.22 **ATOM** 527 C ILE 275 45.175 3.032 10.086 1.00 51.78 **ATOM** 528 O ILE 275 44.578 3.108 11.159 1.00 49.80 529 N ILE **ATOM** 276 45.710 4.088 9.481 1.00 51.76 **ATOM 530 CA ILE** 276 45.657 5.416 10.084 1.00 52.58 **ATOM** 531 CB ILE 276 46.733 6.364 9.464 1.00 55.04 **ATOM** 532 CG2 ILE 276 46.395 6.696 8.020 1.00 53.28 46.823 **ATOM** 533 CG1 ILE 276 7.663 10.270 1.00 57.31 **ATOM** 534 CD1 ILE 276 47.364 7.485 11.664 1.00 60.32 **ATOM** 535 C ILE 276 44.279 6.073 9.974 1.00 50.70 ATOM 536 O ILE 276 43.858 6.775 10.895 1.00 55.55

ATOM 537 N THR 277 8.866 1.00 47.33 43.576 5.849 **ATOM** 538 CA THR 277 42.255 6.450 8.681 1.00 42.59 **ATOM** 539 CB THR 277 41.695 6.190 7.254 1.00 44.97 **ATOM** 540 OG1 THR 277 42.611 6.702 6.280 1.00 46.38 **ATOM** 541 CG2 THR 277 40.349 6.892 7.065 1.00 37.17 542 C- THR 277 **ATOM** 41.252 5.954 9.718 1.00 39.84 543 O THR **ATOM** 277 40.570 6.759 10.351 1.00 40.55 **ATOM** 544 N PRO 278 41.126 4.620 9.899 1.00 38.20 **ATOM** 545 CD PRO 278 41.746 3.457 9.242 1.00 36.34 **ATOM** 546 CA PRO 278 40.165 4.167 10.907 1.00 36.63 **ATOM** 547 CB PRO 278 40.242 2.639 10.783 1.00 32.95 **ATOM** 548 CG PRO 278 41.668 2.419 10.343 1.00 35.75 **ATOM** 549 C PRO 278 40.532 4.681 12.306 1.00 38.60 **ATOM** 550 O PRO 278 39.653 5.017 13.104 1.00 37.67 **ATOM** 551 N ALA 279 41.831 4.758 12.586 1.00 37.05 **ATOM** 552 CA ALA 279 42.315 5.248 13.877 1.00 33.18 **ATOM** 553 CB ALA 279 43.836 5.135 13.949 1.00 30.56 **ATOM** 554 C ALA 279 41.890 6.692 14.077 1.00 33.47 **ATOM** 555 O ALA 279 41.403 7.060 15.151 1.00 33.74 **ATOM** 556 N ILE 280 42.067 7.517 13.041 1.00 29.96 **ATOM** 557 CA ILE 280 41.687 8.921 13.121 1.00 25.94 **ATOM** 558 CB ILE 280 42.155 9.716 11.871 1.00 26.95 **ATOM** 559 CG2 ILE 280 41.643 11.168 11.923 1.00 15.40 ATOM 560 CG1 ILE 280 43.686 9.702 11.798 1.00 26.73 **ATOM** 561 CD1 ILE 280 44.255 10.378 10.550 1.00 34.31 **ATOM** 562 C ILE 280 40.181 9.074 13.251 1.00 31.39 563 O ILE 280 **ATOM** 39.696 9.943 13.973 1.00 35.69 564 N THR 281 **ATOM** 39.428 8.226 12.552 1.00 30.90 **ATOM** 565 CA THR 281 37.982 8.318 12.592 1.00 33.49 566 CB THR 281 **ATOM** 37.321 7.451 11.478 1.00 37.18 **ATOM** 567 OG1 THR 281 37.760 6.091 11.592 1.00 46.48 **ATOM** 568 CG2 THR 281 37.703 7.972 10.114 1.00 32.85 569 C THR 281 **ATOM** 37.435 7.926 13.968 1.00 29.94 **ATOM** 570 O THR 281 36.428 8.473 14.408 1.00 25.55 282 **ATOM** 571 N ARG 38.103 6.997 14.641 1.00 32.70 **ATOM** 572 CA ARG 282 37.676 6.585 15.975 1.00 34.27 **ATOM** 573 CB ARG 282 38.511 5.411 16.479 1.00 33.78 **ATOM** 574 CG ARG 282 38.259 4.111 15.743 1.00 45.15 **ATOM** 575 CD ARG 282 39.017 2.976 16.404 1.00 58.24 **ATOM** 576 NE ARG 282 38.763 1.679 15.776 1.00 68.41 39.141 1.344 14.546 1.00 72.31 **ATOM** 577 CZ ARG 282 **ATOM** 578 NH1 ARG 282 39.802 2.213 13.791 1.00 77.89 **ATOM** 579 NH2 ARG 282 38.864 0.139 14.066 1.00 69.25 **ATOM** 37.789 7.764 16.942 1.00 34.81 580 C ARG 282 **ATOM** 581 O ARG 282 37.006 7.886 17.884 1.00 36.03 **ATOM** 38.761 8.640 16.696 1.00 31.71 582 N VAL 283

ATOM 583 CA VAL 283 38.952 9.815 17.532 1.00 30.16 **ATOM** 584 CB VAL 40.298 10.524 17.224 1.00 29.00 283 **ATOM** 585 CG1 VAL 283 40.448 11.777 18.076 1.00 28.64 **ATOM** 586 CG2 VAL 283 41.448 9.577 17.487 1.00 28.28 **ATOM** 587 C VAL 283 37.801 10.787 17.292 1.00 32.50 **ATOM** 588 O. VAL 283 37.284 11.388 18.236 1.00 33.48 **ATOM** 589 N VAL 284 37.403 10.945 16.028 1.00 30.96 **ATOM** 590 CA VAL 284 36.293 11.838 15.694 1.00 29.14 **ATOM** 591 CB VAL 284 36.138 12.023 14.158 1.00 31.27 **ATOM** 592 CG1 VAL 284 34.990 12.985 13.868 1.00 24.21 **ATOM** 593 CG2 VAL 284 37.450 12.565 13.554 1.00 30.51 **ATOM** 594 C VAL 284 34.995 11.260 16.258 1.00 28.89 **ATOM** 595 O VAL 284 34.146 12.005 16.743 1.00 27.29 **ATOM** 596 N ASP 285 34.845 9.937 16.208 1.00 28.76 **ATOM** 597 CA ASP 285 33.639 9.307 16.738 1.00 35.32 **ATOM** 598 CB ASP 285 33.627 7.792 16.459 1.00 33.29 **ATOM** 599 CG ASP 285 33.523 7.471 14.971 1.00 38.15 ATOM 600 OD1 ASP 285 32.729 8.139 14.276 1.00 34.70 **ATOM** 601 OD2 ASP 285 34.209 6.532 14.504 1.00 34.43 **ATOM** 602 C ASP 285 33.531 9.553 18.248 1.00 36.70 **ATOM** 603 O **ASP** 285 32.431 9.685 18.786 1.00 37.96 **ATOM** 604 N PHE 286 34.679 9.624 18.916 1.00 35.96 286 **ATOM** 605 CA PHE 34.736 9.869 20.349 1.00 37.10 **ATOM** 606 CB PHE 286 36.187 9.777 20.845 1.00 37.97 **ATOM** 607 CG PHE 286 36.377 10.219 22.283 1.00 36.50 **ATOM** 608 CD1 PHE 286 35.815 9.490 23.340 1.00 36.75 **ATOM** 609 CD2 PHE 286 37.100 11.381 22.575 1.00 33.83 **ATOM** 610 CE1 PHE 286 35.966 9.917 24.685 1.00 39.55 **ATOM** 611 CE2 PHE 286 37.265 11.831 23.911 1.00 38.08 **ATOM** 612 CZ PHE 286 36.696 11.092 24.972 1.00 34.44 **ATOM** 613 C PHE 286 34.179 11.249 20.665 1.00 36.83 614 O PHE **ATOM** 286 33.292 11.401 21.518 1.00 35.61 **ATOM** 615 N ALA 287 34.696 12.255 19.968 1.00 37.33 **ATOM** 616 CA ALA 287 34.266 13.631 20.171 1.00 36.34 **ATOM** 617 CB ALA 287 35.118 14.565 19.325 1.00 36.40 **ATOM** 618 C ALA 287 32.785 13.840 19.861 1.00 38.76 619 O ALA 287 **ATOM** 32.121 14.641 20.525 1.00 41.98 **ATOM** 620 N LYS 288 32.267 13.130 18.862 1.00 38.28 **ATOM** 621 CA LYS 288 30.856 13.268 18.499 1.00 45.26 **ATOM** 622 CB LYS 288 30.541 12.534 17.188 1.00 48.35 **ATOM** 623 CG LYS 288 31.159 13.158 15.951 1.00 51.43 **ATOM** 624 CD LYS 288 30.556 12.589 14.665 1.00 60.23 625 CE LYS **ATOM** 288 30.848 11.107 14.479 1.00 62.81 626 NZ LYS 288 **ATOM** 32.312 10.852 14.392 1.00 64.69 **ATOM** 627 C LYS 288 29.913 12.763 19.586 1.00 43.31 **ATOM** 628 O LYS 288 28.791 13.253 19.707 1.00 45.66

ATOM .629 N LYS 289 30.367 11.789 20.371 1.00 41.70 ATOM 630 CA LYS 289 29.548 11.235 21.443 1.00 40.67 **ATOM** 631 CB LYS 289 29.984 9.806 21.767 1.00 42.25 632 CG LYS **ATOM** 289 29.912 8.853 20.591 1.00 39.53 **ATOM** 633 CD LYS 289 30.341 7.456 21.003 1.00 43.19 **ATOM** 634 CE LYS 289 30.454 6.539 19.807 1.00 45.74 **ATOM** 635 NZ LYS 289 29.175 6.457 19.049 1.00 52.49 **ATOM** 636 C LYS 289 29.585 12.076 22.721 1.00 41.50 **ATOM** 637 O LYS 289 29.030 11.676 23.742 1.00 39.77 **ATOM** 638 N LEU 290 30.242 13.235 22.661 1.00 40.68 **ATOM** 639 CA LEU 290 30.307 14.143 23.811 1.00 39.33 **ATOM** 640 CB LEU 290 31.757 14.590 24.075 1.00 36.14 ATOM 641 CG LEU 290 32.815 13.526 24.401 1.00 34.81 **ATOM** 642 CD1 LEU 290 34.155 14.200 24.558 1.00 29.07 **ATOM** 643 CD2 LEU 290 32.445 12.764 25.667 1.00 33.45 ATOM 644 C LEU 290 29.448 15.368 23.481 1.00 40.08 **ATOM** 645 O LEU 290 29.828 16.196 22.655 1.00 42.00 **ATOM** 646 N **PRO** 291 28.279 15.500 24.137 1.00 40.27 **ATOM** 647 CD PRO 291 27.716 14.625 25.185 1.00 39.65 **ATOM** 648 CA PRO 291 27.372 16.628 23.899 1.00 38.28 **ATOM** 649 CB PRO 291 26.327 16.447 24.997 1.00 35.88 **ATOM** 650 CG PRO 291 26.230 14.932 25.071 1.00 34.19 ATOM 651 C **PRO** 291 28.010 18.006 23.910 1.00 40.05 **ATOM** 652 O **PRO** 291 27.663 18.857 23.089 1.00 41.33 **ATOM** 653 N **MET** 292 28.933 18.235 24.837 1.00 40.59 **ATOM** 654 CA MET 292 29.607 19.529 24.932 1.00 42.86 **ATOM** 655 CB MET 292 30.635 19.521 26.059 1.00 43.28 **ATOM** 656 CG MET 292 30.050 19.286 27.428 1.00 50.35 **ATOM 657 SD MET** 292 31.329 19.157 28.679 1.00 51.17 ATOM 658 CE MET 292 30.331 18.787 30.111 1.00 54.63 **ATOM** 659 C **MET** 292 30.311 19.869 23.629 1.00 41.05 **ATOM MET** 292 660 O 30.341 21.024 23.210 1.00 39.66 **ATOM** 661 N PHE 293 30.882 18.854 22.992 1.00 39.30 **ATOM** 662 CA PHE 293 31.594 19.057 21.747 1.00 40.92 **ATOM** 663 CB PHE 293 32.300 17.772 21.335 1.00 40.98 **ATOM** 664 CG PHE 293 33.117 17.902 20.070 1.00 42.78 **ATOM** 665 CD1 PHE 293 34.272 18.692 20.046 1.00 44.40 666 CD2 PHE 32.727 17.235 18.902 1.00 43.66 **ATOM** 293 **ATOM** 667 CE1 PHE 293 35.051 18.823 18.865 1.00 39.83 **ATOM** 668 CE2 PHE 293 33.483 17.348 17.710 1.00 46.21 **ATOM** 669 CZ PHE 293 34.654 18.147 17.693 1.00 45.18 **ATOM** 293 670 C PHE 30.653 19.492 20.624 1.00 45.54 **ATOM** PHE 671 O 293 30.985 20.377 19.829 1.00 42.01 **ATOM** 672 N **CYS** 294 29.468 18.895 20.579 1.00 47.05 **ATOM** 673 CA CYS 294 28.545 19.200 19.512 1.00 50.15 27.320 18.329 19.584 1.00 45.90 **ATOM** 674 CB CYS 294

ATOM .675 SG CYS 294 27.680 16.529 19.352 1.00 51.50 **ATOM** 676 C CYS 294 28.062 20.636 19.582 1.00 51.38 **ATOM** 677 O **CYS** 294 27.682 21.199 18.543 1.00 53.83 **ATOM** 678 N GLU 295 27.996 21.170 20.802 1.00 49.72 **ATOM** 679 CA GLU 295 27.541 22.535 21.067 1.00 52.53 **ATOM** 680 CB GLU 27.384 22.762 22.575 1.00 57.40 295 **ATOM** 681 CG GLU 295 26.179 22.090 23.208 1.00 69.63 **ATOM** 682 CD GLU 295 24.871 22.731 22.785 1.00 78.49 **ATOM** 683 OE1 GLU 295 24.698 23.942 23.041 1.00 82.82 **ATOM** 684 OE2 GLU 295 24.017 22.029 22.199 1.00 85.30 **ATOM** 685 C GLU 295 28.484 23.589 20.515 1.00 48.54 **ATOM** 686 O **GLU** 295 28.170 24.777 20.537 1.00 49.82 **ATOM** 687 N LEU 296 29.637 23.149 20.030 1.00 43.79 **ATOM** 688 CA LEU 296 30.629 24.066 19.476 1.00 45.42 **ATOM** 689 CB LEU 296 32.040 23.541 19.771 1.00 41.04 **ATOM** 690 CG LEU 296 32.416 23.394 21.252 1.00 42.74 **ATOM** 691 CD1 LEU 296 33.789 22.753 21.352 1.00 40.99 **ATOM** 692 CD2 LEU 296 32.406 24.755 21.945 1.00 39.44 **ATOM** 693 C LEU 296 30.448 24.239 17.968 1.00 45.56 **ATOM** 694 O LEU 296 29.966 23.333 17.278 1.00 43.07 **ATOM** 695 N PRO 297 30.823 25.414 17.436 1.00 46.99 **ATOM** 696 CD PRO 297 31.372 26.613 18.083 1.00 47.12 697 CA PRO **ATOM** 297 30.689 25.650 15.998 1.00 49.61 **ATOM** 698 CB PRO 297 31.106 27.118 15.861 1.00 49.91 **ATOM** 699 CG PRO 297 30.757 27.693 17.230 1.00 51.28 **ATOM** 700 C PRO 297 31.600 24.717 15.202 1.00 49.59 **ATOM** 701 O PRO 297 32.727 24.446 15.615 1.00 51.66 702 N CYS 31.093 24.227 14.075 1.00 51.02 **ATOM** 298 **ATOM** 703 CA CYS 298 31.817 23.322 13.158 1.00 52.86 **ATOM** 704 CB CYS 298 31.100 23.260 11.804 1.00 54.57 **ATOM** 705 SG CYS 298 31.935 24.249 10.470 1.00 67.87 **ATOM** 706 C CYS 298 33.269 23.797 12.974 1.00 48.51 **ATOM** 707 O **CYS** 298 34.197 22.991 12.819 1.00 49.58 **ATOM** 708 N GLU 299 33.464 25.113 13.019 1.00 44.17 **ATOM** 709 CA GLU 299 34.797 25.692 12.890 1.00 47.57 **ATOM** 710 CB GLU 299 34.741 27.227 12.912 1.00 49.92 **ATOM** 299 34.001 27.871 11.747 1.00 59.30 711 CG GLU **ATOM** 712 CD GLU 299 32.489 27.763 11.848 1.00 63.80 299 **ATOM** 713 OE1 GLU 31.805 28.162 10.882 1.00 69.03 **ATOM** 714 OE2 GLU 299 31.979 27.297 12.889 1.00 67.10 **ATOM** 715 C GLU 299 35.698 25.213 14.031 1.00 46.57 **ATOM** GLU 299 716 O 36.772 24.659 13.787 1.00 44.65 **ATOM** 717 N ASP 300 35.263 25.432 15.274 1.00 45.17 **ATOM** 718 CA ASP 300 36.046 25.008 16.433 1.00 43.32 **ATOM** 719 CB ASP 300 35.442 25.517 17.747 1.00 37.38 **ATOM** 300 **720 CG ASP** 35.567 27.016 17.910 1.00 36.23

380

ATOM .721 OD1 ASP 300 36.486 27.613 17.313 1.00 35.87 **ATOM** 722 OD2 ASP 300 34.769 27.601 18.669 1.00 40.14 **ATOM** 723 C ASP 300 36.174 23.495 16.513 1.00 42.81 **ATOM** 724 O ASP 300 37.193 22.979 16.974 1.00 46.02 **ATOM** 725 N GLN 301 35.139 22.788 16.066 1.00 38.60 **ATOM 726 CA GLN** 301 35.151 21.334 16.086 1.00 40.00 **ATOM** 727 CB GLN 301 33.815 20.783 15.576 1.00 38.59 **ATOM 728 CG GLN** 301 32.608 21.334 16.317 1.00 40.26 **ATOM** 729 CD GLN 301 31.311 20.696 15.869 1.00 44.15 **ATOM** 730 OE1 GLN 31.074 20.527 14.673 1.00 45.73 301 **ATOM** 731 NE2 GLN 301 30.450 20.363 16.824 1.00 46.13 **ATOM** 732 C GLN 301 36.298 20.807 15.227 1.00 41.64 733 O GLN 301 36.975 19.850 15.601 1.00 45.02 ATOM **ATOM** 734 N ILE 302 36.523 21.441 14.077 1.00 41.01 **ATOM 735 CA ILE** 302 37.607 21.029 13.189 1.00 40.23 **ATOM 736 CB ILE** 302 37.580 21.798 11.825 1.00 39.52 **ATOM** 737 CG2 ILE 302 38.724 21.308 10.931 1.00 31.98 **ATOM** 738 CG1 ILE 302 36.230 21.607 11.119 1.00 40.77 **ATOM** 739 CD1 ILE 302 35.895 20.166 10.733 1.00 45.43 **ATOM** 740 C ILE 302 38.948 21.322 13.869 1.00 38.58 **ATOM** 741 O ILE 302 39.811 20.452 13.938 1.00 40.81 **ATOM** 742 N ILE 303 39.110 22.547 14.364 1.00 37.50 743 CA ILE ATOM 303 40.343 22.958 15.030 1.00 39.33 **ATOM** 744 CB ILE 303 40.263 24.442 15.501 1.00 39.06 **ATOM** 745 CG2 ILE 303 41.525 24.822 16.279 1.00 36.19 **ATOM** 746 CG1 ILE 303 40.103 25.358 14.280 1.00 40.15 **ATOM** 747 CD1 ILE 303 39.972 26.846 14.602 1.00 36.93 **ATOM** 748 C ILE 303 40.676 22.061 16.222 1.00 36.49 **ATOM** 749 O ILE 303 41.818 21.623 16.378 1.00 36.58 750 N LEU ATOM 304 39.674 21.788 17.057 1.00 32.91 **ATOM** 751 CA LEU 304 39.851 20.940 18.234 1.00 27.55 **ATOM** 752 CB LEU 304 38.546 20.875 19.026 1.00 22.35 **ATOM 753 CG LEU** 304 38.472 21.629 20.361 1.00 26.88 **ATOM** 754 CD1 LEU 304 39.096 22.998 20.275 1.00 24.82 **ATOM** 755 CD2 LEU 304 37.024 21.728 20.787 1.00 23.69 **ATOM** 756 C LEU 304 40.313 19.534 17.855 1.00 28.05 **ATOM** 757 O LEU 304 41.277 19.013 18.429 1.00 24.68 **ATOM** 758 N LEU 305 39.637 18.929 16.882 1.00 26.34 **ATOM 759 CA LEU** 305 39.997 17.588 16.436 1.00 30.91 **ATOM** 760 CB LEU 305 38.937 17.055 15.466 1.00 32.50 **ATOM** 761 CG LEU 305 37.585 16.757 16.132 1.00 33.36 762 CD1 LEU **ATOM** 305 36.557 16.439 15.079 1.00 33.87 **ATOM** 763 CD2 LEU 305 37.733 15.581 17.101 1.00 31.72 **ATOM** 764 C LEU 305 41.381 17.523 15.796 1.00 29.76 **ATOM** 765 O LEU 305 42.109 16.553 15.990 1.00 29.33 **ATOM** 766 N LYS 306 41.754 18.554 15.048 1.00 29.72

ATOM 767 CA LYS 306 43.065 18.569 14.409 1.00 34.28 **ATOM** 768 CB LYS 306 43.122 19.673 13.345 1.00 35.98 **ATOM 769 CG LYS** 306 42.140 19.465 12.206 1.00 43.35 **ATOM** 770 CD LYS 306 42.195 20.583 11.170 1.00 51.50 **ATOM** 771 CE LYS 306 43.532 20.639 10.446 1.00 53.26 **ATOM** 772 NZ LYS 306 43.522 21.702 9.409 1.00 59.61 **ATOM** 773 C LYS 306 44.183 18.777 15.434 1.00 35.25 **ATOM** 774 O LYS 306 45.312 18.332 15.231 1.00 33.95 **ATOM** 775 N GLY 307 43.853 19.446 16.536 1.00 35.79 **ATOM** 776 CA GLY 307 44.836 19.700 17.576 1.00 34.59 **ATOM** 777 C **GLY** 307 45.075 18.562 18.559 1.00 33.80 **ATOM** 778 O **GLY** 307 46.200 18.360 19.008 1.00 31.59 **ATOM** 779 N CYS 308 44.030 17.806 18.880 1.00 31.15 **ATOM** 780 CA CYS 308 44.153 16.712 19.839 1.00 29.04 **ATOM** 308 **781 CB CYS** 42.929 16.667 20.750 1.00 27.59 **ATOM** 782 SG CYS 308 41.452 15.974 19.941 1.00 30.50 **ATOM** 783 C CYS 308 44.289 15.339 19.208 1.00 30.59 **ATOM** 784 O **CYS** 308 44.609 14.374 19.899 1.00 33.77 **ATOM** 785 N CYS 309 44.053 15.247 17.907 1.00 28.46 **ATOM** 786 CA CYS 309 44.099 13.961 17.219 1.00 30.10 **ATOM** 787 CB CYS 309 43.983 14.161 15.706 1.00 33.43 **ATOM** 788 SG CYS 309 43.761 12.613 14.819 1.00 35.20 **ATOM** 45.301 13.071 17.524 1.00 27.72 789 C CYS 309 790 O **ATOM CYS** 309 45.135 11.907 17.913 1.00 27.69 **ATOM** 791 N MET 46.508 13.594 17.339 1.00 26.15 310 **ATOM 792 CA MET** 47.700 12.798 17.605 1.00 26.06 310 **ATOM 793 CB MET** 48.928 13.439 16.951 1.00 25.32 310 **ATOM 794 CG MET** 310 50.207 12.648 17.132 1.00 24.08 **ATOM** 795 SD MET 310 50.101 10.991 16.423 1.00 27.71 **ATOM 796 CE MET** 310 51.674 10.307 16.934 1.00 28.50 **ATOM** 797 C MET 310 47.941 12.612 19.113 1.00 25.94 **ATOM** 798 O MET 310 48.592 11.653 19.526 1.00 28.09 **ATOM** 799 N GLU 311 47.405 13.522 19.923 1.00 25.39 **ATOM** 800 CA GLU 311 47.560 13.445 21.370 1.00 27.03 **ATOM** 801 CB GLU 311 47.099 14.748 22.030 1.00 24.39 **ATOM** 802 CG GLU 311 47.610 15.999 21.331 1.00 26.00 803 CD GLU **ATOM** 311 47.292 17.271 22.084 1.00 23.95 **ATOM** 804 OE1 GLU 311 46.182 17.379 22.640 1.00 19.72 **ATOM** 805 OE2 GLU 311 48.150 18.181 22.088 1.00 26.51 **ATOM** 806 C GLU 311 46.727 12.272 21.902 1.00 27.51 **ATOM** 807 O GLU 311 47.152 11.552 22.807 1.00 29.67 **ATOM** 808 N ILE 312 45.547 12.086 21.326 1.00 26.82 809 CA ILE **ATOM** 312 44.661 11.001 21.724 1.00 25.71 810 CB ILE **ATOM** 312 43.194 11.296 21.304 1.00 23.35 **ATOM** 811 CG2 ILE 312 42.301 10.068 21.583 1.00 20.27 **ATOM** 812 CG1 ILE 312 42.690 12.534 22.062 1.00 20.88

ATOM .813 CD1 ILE 312 41.244 12.961 21.755 1.00 18.15 **ATOM** 814 C ILE 312 45.116 9.665 21.132 1.00 27.91 815 O **ATOM** ILE 312 45.064 8.628 21.804 1.00 28.96 **ATOM** 816 N **MET** 313 45.582 9.683 19.886 1.00 27.66 817 CA MET **ATOM** 313 46.045 8.447 19.257 1.00 30.18 **ATOM** 818 CB MET 46.386 313 8.662 17.771 1.00 36.89 **ATOM** 819 CG MET 313 45.186 8.938 16.861 1.00 37.95 ATOM 820 SD MET 313 45.624 8.943 15.096 1.00 42.38 **ATOM** 821 CE MET 313 46.724 10.319 14.999 1.00 40.68 **ATOM** 822 C **MET** 313 47.264 7.897 19.975 1.00 27.43 **ATOM** 823 O **MET** 313 47.351 6.690 20.219 1.00 28.61 **ATOM** 824 N SER 314 48.202 8.776 20.318 1.00 24.88 **ATOM** 825 CA SER 314 49.416 8.352 21.011 1.00 27.98 **ATOM** 826 CB SER 314 50.420 9.511 21.118 1.00 29.64 314 **ATOM** 827 OG SER 49.912 10.560 21.911 1.00 43.44 **ATOM** 828 C SER 49.082 7.818 22.402 1.00 22.30 314 **ATOM** 829 O SER 314 49.737 6.895 22.892 1.00 24.18 **ATOM** 830 N LEU 315 48.070 8.395 23.039 1.00 23.99 831 CA LEU 315 47.646 7.918 24.365 1.00 25.07 **ATOM** 832 CB LEU **ATOM** 315 46.580 8.842 24.965 1.00 19.11 833 CG LEU **ATOM** 315 45.863 8.355 26.228 1.00 20.39 **ATOM** 834 CD1 LEU 315 46.872 8.076 27.362 1.00 18.92 **ATOM** 835 CD2 LEU 315 44.848 9.401 26.655 1.00 12.93 **ATOM** 836 C LEU 315 47.070 6.518 24.222 1.00 24.53 **ATOM** 837 O LEU 315 47.394 5.615 24.992 1.00 26.32 46.212 **ATOM** 838 N ARG 316 6.338 23.220 1.00 28.18 **ATOM** 839 CA ARG 316 45.595 5.041 22.978 1.00 27.54 840 CB ARG **ATOM** 316 44.575 5.155 21.848 1.00 27.39 **ATOM** 841 CG ARG 316 43.340 5.929 22.253 1.00 22.00 **ATOM** 842 CD ARG 5.902 21.172 1.00 18.78 316 42.291 **ATOM** 843 NE ARG 316 40.975 6.205 21.719 1.00 26.57 **ATOM** 844 CZ ARG 316 39.852 6.224 21.014 1.00 30.81 **ATOM** 845 NH1 ARG 316 39.878 5.972 19.711 1.00 33.71 **ATOM** 846 NH2 ARG 316 38.692 6.471 21.613 1.00 33.13 **ATOM** 847 C ARG 316 46.612 3.949 22.682 1.00 28.09 **ATOM** 848 O ARG 316 46.399 2.790 23.027 1.00 32.41 849 N ALA 317 **ATOM** 47.718 4.317 22.047 1.00 28.36 **ATOM** 850 CA ALA 317 48.771 3.359 21.744 1.00 26.64 **ATOM** 851 CB ALA 317 49.674 3.904 20.643 1.00 22.93 **ATOM** 852 C ALA 317 49.591 3.115 23.002 1.00 28.35 **ATOM** 853 O ALA 317 49.968 1.979 23.312 1.00 32.10 **ATOM** 854 N ALA 318 49.863 4.197 23.727 1.00 29.12 **ATOM** 855 CA ALA 318 50.655 4.123 24.953 1.00 27.50 **ATOM** 856 CB ALA 50.854 5.518 25.522 1.00 28.39 318 **ATOM** 857 C ALA 318 50.053 3.215 26.013 1.00 28.10 50.783 **ATOM** 858 O ALA 318 2.491 26.684 1.00 28.18

ATOM	859 N VAL 319	48.730 3.245 26.165 1.00 29.16
ATOM	860 CA VAL 319	48.082 2.414 27.176 1.00 35.24
ATOM	861 CB VAL 319	46.663 2.933 27.541 1.00 27.34
ATOM	862 CG1 VAL 319	46.759 4.324 28.136 1.00 29.96
ATOM	863 CG2 VAL 319	45.773 2.936 26.322 1.00 31.70
ATOM	864 C · VAL 319	47.970 0.955 26.764 1.00 40.01
ATOM	865 O VAL 319	47.448 0.129 27.515 1.00 42.70
ATOM	866 N ARG 320	48.460 0.644 25.565 1.00 38.64
ATOM	867 CA ARG 320	48.436 -0.715 25.041 1.00 38.61
ATOM	868 CB ARG 320	47.764 -0.751 23.674 1.00 37.26
ATOM	869 CG ARG 320	46.258 -0.655 23.720 1.00 43.12
ATOM	870 CD ARG 320	45.712 -0.368 22.339 1.00 50.79
ATOM	871 NE ARG 320	44.260 -0.446 22.286 1.00 54.71
ATOM	872 CZ ARG 320	43.527 0.074 21.306 1.00 57.89
ATOM	873 NH1 ARG 320	44.119 0.713 20.300 1.00 49.08
ATOM	874 NH2 ARG 320	42.206 -0.058 21.326 1.00 59.59
ATOM	875 C ARG 320	49.852 -1.247 24.930 1.00 42.14
ATOM	876 O ARG 320	50.162 -2.055 24.051 1.00 46.30
ATOM	877 N TYR 321	50.712 -0.772 25.822 1.00 42.04
ATOM	878 CA TYR 321	52.098 -1.202 25.852 1.00 42.70
ATOM	879 CB TYR 321	52.971 -0.133 26.529 1.00 38.01
ATOM	880 CG TYR 321	54.416 -0.579 26.734 1.00 37.94
ATOM	881 CD1 TYR 321	55.275 -0.779 25.636 1.00 33.85
ATOM	882 CE1 TYR 321	56.581 -1.297 25.813 1.00 34.49
ATOM	883 CD2 TYR 321	54.892 -0.894 28.016 1.00 28.03
ATOM	884 CE2 TYR 321	56.194 -1.411 28.207 1.00 32.69
ATOM	885 CZ TYR 321	57.026 -1.614 27.103 1.00 35.18
ATOM	886 OH TYR 321	58.289 -2.158 27.288 1.00 39.48
ATOM	887 C TYR 321	52.189 -2.515 26.629 1.00 45.51
ATOM	888 O TYR 321	51.571 -2.662 27.687 1.00 48.02
ATOM	889 N ASP 322	52.945 -3.471 26.095 1.00 44.56
ATOM	890 CA ASP 322	53.129 -4.764 26.753 1.00 45.86
ATOM	891 CB ASP 322	52.697 -5.899 25.816 1.00 46.64
ATOM	892 C ASP 322	54.606 -4.910 27.098 1.00 45.82
ATOM	893 O ASP 322 894 N PRO 323	55.434 -5.109 26.214 1.00 45.38
ATOM ATOM		54.962 -4.803 28.393 1.00 46.53
ATOM	895 CD PRO 323 896 CA PRO 323	54.123 -4.541 29.572 1.00 47.16 56.366 -4.932 28.805 1.00 46.63
ATOM	897 CB PRO 323	56.293 -4.667 30.308 1.00 43.95
ATOM	898 CG PRO 323	54.926 -5.223 30.655 1.00 43.93
ATOM	899 C PRO 323	56.993 -6.285 28.478 1.00 48.34
ATOM	900 O PRO 323	58.217 -6.407 28.379 1.00 50.84
ATOM	901 N GLU 324	56.149 -7.301 28.315 1.00 52.39
ATOM	902 CA GLU 324	56.621 -8.646 28.005 1.00 55.85
ATOM	903 CB GLU 324	55.453 -9.633 28.048 1.00 55.54
ATOM	904 C GLU 324	57.283 -8.670 26.632 1.00 54.94
	20. 0 000 00	

ATOM 905 O GLU 324 58.460 -9.013 26.502 1.00 59.81 **ATOM** 906 N SER 325 56.522 -8.299 25.611 1.00 52.95 **ATOM** 907 CA SER 325 57.021 -8.269 24.244 1.00 50.10 **ATOM** 908 CB SER 325 55.889 -8.613 23.279 1.00 48.23 **ATOM** 909 OG SER 325 54.788 -7.749 23.471 1.00 48.71 ATOM 910 C. SER 325 57.608 -6.908 23.879 1.00 50.61 **ATOM** 911 O SER 325 58.194 -6.743 22.808 1.00 52.19 **ATOM** 912 N GLU 326 57.450 -5.939 24.786 1.00 45.64 **ATOM** 913 CA GLU 326 57.938 -4.579 24.588 1.00 43.35 **ATOM** 914 CB GLU 326 59.469 -4.562 24.587 1.00 42.74 **ATOM** 915 CG GLU 326 60.053 -5.016 25.909 1.00 50.32 **ATOM** 916 CD GLU 326 61.565 -5.067 25.907 1.00 56.34 **ATOM** 917 OE1 GLU 326 62.139 -5.407 26.966 1.00 59.31 **ATOM** 918 OE2 GLU 326 62.178 -4.774 24.856 1.00 55.74 **ATOM** 919 C GLU 326 57.397 -3.993 23.291 1.00 40.23 **ATOM** 920 O GLU 326 58.145 -3.474 22.465 1.00 40.44 **ATOM** 921 N THR 327 56.080 -4.079 23.127 1.00 35.90 922 CA THR 327 **ATOM** 55.427 -3.573 21.936 1.00 37.29 **ATOM** 923 CB THR 327 54.983 -4.717 21.008 1.00 37.63 924 OG1 THR 327 **ATOM** 53.994 -5.503 21.674 1.00 38.12 **ATOM** 925 CG2 THR 327 56.165 -5.609 20.635 1.00 39.90 **ATOM** 926 C THR 327 54.170 -2.780 22.282 1.00 39.49 THR **ATOM** 927 O 327 53.603 -2.930 23.364 1.00 40.50 928 N LEU 328 **ATOM** 53.758 -1.933 21.347 1.00 36.64 **ATOM** 929 CA LEU 328 52.544 -1.136 21.480 1.00 37.73 **ATOM** 930 CB LEU 328 52.791 0.340 21.127 1.00 37.78 **ATOM** 931 CG LEU 328 53.667 1.257 21.982 1.00 36.26 932 CD1 LEU **ATOM** 328 53.690 2.641 21.348 1.00 36.56 **ATOM** 933 CD2 LEU 328 53.101 1.351 23.396 1.00 39.85 **ATOM** 934 C LEU 328 51.617 -1.722 20.431 1.00 37.27 **ATOM** 935 O LEU 328 52.083 -2.233 19.410 1.00 34.96 **ATOM** 936 N THR 329 50.314 -1.652 20.669 1.00 39.73 **ATOM** 937 CA THR 329 49.368 -2.173 19.701 1.00 40.81 ATOM 938 CB THR 329 48.401 -3.176 20.349 1.00 42.67 **ATOM** 939 OG1 THR 329 49.156 -4.271 20.896 1.00 42.52 940 CG2 THR **ATOM** 329 47.425 -3.722 19.315 1.00 43.52 941 C THR **ATOM** 329 48.591 -1.034 19.058 1.00 44.31 **ATOM** 942 O THR 329 47.825 -0.325 19.712 1.00 43.72 **ATOM** 943 N LEU 330 48.822 -0.859 17.759 1.00 44.62 **ATOM** 944 CA LEU 330 48.179 0.182 16.972 1.00 45.09 **ATOM** 945 CB LEU 330 49.056 0.545 15.766 1.00 44.66 **ATOM** 946 CG LEU 330 50.329 1.393 15.951 1.00 51.06 **ATOM** 947 CD1 LEU 330 51.195 0.890 17.095 1.00 48.58 948 CD2 LEU **ATOM** 330 51.107 1.387 14.638 1.00 45.18 **ATOM** 949 C LEU 330 46.802 -0.264 16.501 1.00 48.06 **ATOM** 950 O LEU 330 46.634 -1.386 16.012 1.00 49.33

ATOM 951 N ASN 45.826 331 0.618 16.663 1.00 52.20 **ATOM** 952 CA ASN 331 44.450 0.363 16.257 1.00 54.41 **ATOM** 953 CB ASN 331 44.370 0.353 14.731 1.00 54.94 954 CG ASN **ATOM** 331 42.970 0.603 14.219 1.00 60.35 **ATOM** 955 OD1 ASN 331 42.375 1.642 14.501 1.00 61.84 **ATOM** 956 ND2 ASN 331 42.438 -0.344 13.459 1.00 65.92 **ATOM** 957 C ASN 43.940 -0.963 16.836 1.00 58.00 331 **ATOM** 958 O ASN 331 42.985 -1.557 16.328 1.00 60.17 **ATOM** 959 N GLY 332 44.590 -1.414 17.908 1.00 58.45 **ATOM** 960 CA GLY 332 44.215 -2.658 18.556 1.00 58.55 **ATOM** 961 C GLY 332 44.408 -3.880 17.680 1.00 59.79 **ATOM** 962 O GLŸ 332 43.892 -4.953 17.993 1.00 61.32 **ATOM** 963 N GLU 333 45.165 -3.725 16.597 1.00 60.28 **ATOM** 964 CA GLU 333 45.408 -4.821 15.659 1.00 59.13 **ATOM** 965 CB GLU 333 44.817 -4.478 14.293 1.00 62.40 **ATOM** 966 CG GLU 333 43.345 -4.129 14.296 1.00 75.69 **ATOM** 967 CD GLU 333 42.851 -3.731 12.917 1.00 80.41 **ATOM** 968 OE1 GLU 333 43.374 -2.740 12.359 1.00 79.98 **ATOM** 969 OE2 GLU 333 41.942 -4.412 12.392 1.00 83.81 **ATOM** 970 C GLU 333 46.881 -5.146 15.452 1.00 57.18 **ATOM** 971 O **GLU** 333 47.291 -6.301 15.545 1.00 57.50 **ATOM** 972 N MET 334 47.663 -4.112 15.166 1.00 55.20 **ATOM 973 CA MET** 334 49.085 -4.245 14.873 1.00 50.85 **ATOM 974 CB MET** 334 49.416 -3.334 13.687 1.00 48.70 **ATOM 975 CG MET** 334 50.844 -3.412 13.181 1.00 45.39 **ATOM** 976 SD MET 334 51.159 -2.124 11.959 1.00 44.56 **ATOM 977 CE MET** 334 49.908 -2.477 10.749 1.00 45.25 **ATOM** 978 C MET 50.041 -3.941 16.026 1.00 51.59 334 **ATOM** 979 O MET 334 50.104 -2.810 16.508 1.00 52.52 **ATOM** 980 N ALA 335 50.796 -4.946 16.450 1.00 51.00 **ATOM** 981 CA ALA 335 51.769 -4.787 17.527 1.00 48.98 **ATOM** 982 CB ALA 335 51.850 -6.062 18.347 1.00 47.86 **ATOM** 983 C ALA 335 53.136 -4.470 16.917 1.00 51.01 **ATOM** 984 O ALA 335 53.655 -5.242 16.109 1.00 51.61 **ATOM** 985 N VAL 336 53.718 -3.336 17:307 1.00 46.62 **ATOM** 986 CA VAL 336 55.016 -2.926 16.783 1.00 42.35 **ATOM** 987 CB VAL 336 54.876 -1.687 15.877 1.00 42.41 **ATOM** 988 CG1 VAL 336 53.963 -2.004 14.707 1.00 42.00 **ATOM** 989 CG2 VAL 336 54.313 -0.506 16.676 1.00 40.32 **ATOM** 990 C **VAL 336** 56.023 -2.608 17.883 1.00 45.33 **ATOM** 991 O VAL 336 55.650 -2.309 19.019 1.00 47.42 THR **ATOM** 992 N 337 57.310 -2.678 17.541 1.00 41.60 **ATOM** 993 CA THR 337 58.357 -2.381 18.508 1.00 39.69 **ATOM** 994 CB THR 337 59.608 -3.259 18.296 1.00 41.35 **ATOM** 995 OG1 THR 337 60.168 -2.985 17.007 1.00 49.35 **ATOM** 996 CG2 THR 337 59.253 -4.734 18.392 1.00 40.38

ATOM .997 C THR 337 58.777 -0.924 18.367 1.00 37.88 **ATOM** 998 O THR 337 58.312 -0.218 17.473 1.00 34.06 **ATOM** 999 N ARG 338 59.655 -0.489 19.268 1.00 37.61 **ATOM** 1000 CA ARG 338 60.171 0.876 19.268 1.00 38.68 ATOM 1001 CB ARG 338 61.177 1.041 20.424 1.00 35.95 ATOM 1002 CG ARG 338 61.804 2.434 20.570 1.00 38.83 **ATOM** 1003 CD ARG 338 62.791 2.462 21.749 1.00 35.88 **ATOM** 1004 NE ARG 62.114 2.277 23.035 1.00 37.42 338 **ATOM** 1005 CZ ARG 338 61.858 3.256 23.902 1.00 30.20 1006 NH1 ARG 338 ATOM 62.224 4.501 23.636 1.00 27.98 **ATOM** 1007 NH2 ARG 338 61.213 2.992 25.025 1.00 27.40 ATOM 1008 C ARG 338 60.843 1.158 17.925 1.00 38.09 **ATOM** 1009 O ARG 338 60.529 2.142 17.251 1.00 34.12 **ATOM** 1010 N GLY 339 61.755 0.267 17.535 1.00 41.25 **ATOM** 1011 CA GLY 339 62.475 0.416 16.282 1.00 41.35 **ATOM** 1012 C GLY 339 61.594 0.463 15.046 1.00 41.23 ATOM 1013 O GLY 339 61.811 1.288 14.159 1.00 38.30 1014 N GLN ATOM 340 60.594 -0.414 14.982 1.00 38.58 **ATOM** 1015 CA GLN 59.704 -0.449 13.826 1.00 40.79 340 **ATOM** 1016 CB GLN 340 58.757 -1.651 13.911 1.00 40.82 1017 CG GLN ATOM 340 59.450 -2.995 13.944 1.00 41.10 1018 CD GLN ATOM 340 58.468 -4.144 13.890 1.00 48.84 57.529 -4.208 14.679 1.00 50.53 ATOM 1019 OE1 GLN 340 **ATOM** 1020 NE2 GLN 340 58.685 -5.068 12.959 1.00 54.25 **ATOM** 1021 C GLN 340 58.884 0.822 13.679 1.00 41.50 **ATOM** 1022 O GLN 340 58.725 1.342 12.576 1.00 42.72 **ATOM** 1023 N LEU 341 58.360 1.324 14.795 1.00 42.00 1024 CA LEU ATOM 341 57.546 2.532 14.775 1.00 38.10 1025 CB LEU **ATOM** 341 56.868 2.740 16.133 1.00 36.66 **ATOM** 1026 CG LEU 341 55.886 3.914 16.267 1.00 39.94 **ATOM** 1027 CD1 LEU 341 54.711 3.741 15.311 1.00 34.98 **ATOM** 1028 CD2 LEU 341 55.389 3.989 17.700 1.00 40.95 **ATOM** 1029 C LEU 341 58.404 3.743 14.423 1.00 36.37 1030 O LEU **ATOM** 341 57.980 4.620 13.668 1.00 37.89 **ATOM** 1031 N LYS 342 59.616 3.777 14.969 1.00 33.29 **ATOM** 1032 CA LYS 342 60.542 4.872 14.723 1.00 35.17 **ATOM** 1033 CB LYS 342 61.801 4.687 15.582 1.00 34.97 **ATOM** 1034 CG LYS 342 62.764 5.863 15.519 1.00 40.00 **ATOM** 1035 CD LYS 342 63.868 5.739 16.555 1.00 34.48 **ATOM** 1036 CE LYS 342 64.709 7.001 16.596 1.00 37.54 **ATOM** 1037 NZ LYS 342 65.716 6.972 17.689 1.00 42.32 **ATOM** 1038 C LYS 342 60.928 4.970 13.235 1.00 38.29 **ATOM** 1039 O LYS 342 60.621 5.963 12.569 1.00 36.23 **ATOM** 1040 N ASN 343 61.585 3.932 12.721 1.00 39.25 **ATOM** 1041 CA ASN 343 62.014 3.903 11.328 1.00 40.19 ATOM 1042 CB ASN 343 62.808 2.627 11.050 1.00 37.96

ATOM 1043 CG ASN 343 63.937 2.429 12.027 1.00 39.22 **ATOM** 1044 OD1 ASN 343 64.648 3.376 12.374 1.00 42.37 **ATOM** 1045 ND2 ASN 343 64.125 1.197 12.471 1.00 42.19 **ATOM** 1046 C ASN 343 60.831 3.997 10.368 1.00 40.12 1047 O ATOM ASN 343 60.991 4.371 9.208 1.00 36.01 **ATOM** 1048 N. GLY 344 59.645 3.665 10.868 1.00 40.95 **ATOM** 1049 CA GLY 344 58.439 3.721 10.057 1.00 39.25 ATOM 1050 C GLY 344 57.947 5.131 9.772 1.00 38.26 **ATOM** 1051 O **GLY** 344 56.971 5.308 9.044 1.00 35.69 ATOM 1052 N GLY 345 58.604 6.135 10.359 1.00 35.89 ATOM 1053 CA GLY 345 58.212 7.510 10.110 1.00 34.00 **ATOM** 1054 C GLY 345 58.050 8.444 11.300 1.00 38.64 **ATOM** 1055 O **GLY** 345 57.902 9.652 11.116 1.00 38.14 ATOM 1056 N LEU 346 58.085 7.912 12.520 1.00 39.52 **ATOM** 1057 CA LEU 346 57.904 8.761 13.692 1.00 36.05 1058 CB LEU **ATOM** 346 57.039 8.048 14.738 1.00 35.72 ATOM 1059 CG LEU 346 55.561 7.864 14.371 1.00 34.89 **ATOM** 1060 CD1 LEU 346 54.850 7.132 15.494 1.00 44.09 **ATOM** 1061 CD2 LEU 346 54.903 9.213 14.146 1.00 34.84 **ATOM** 1062 C LEU 346 59.189 9.264 14.339 1.00 33.52 **ATOM** 1063 O LEU 346 59.171 10.257 15.066 1.00 35.58 **ATOM** 1064 N GLY 347 60.299 8.595 14.067 1.00 30.47 **ATOM** 1065 CA GLY 347 61.559 9.017 14.661 1.00 33.01 **ATOM** 1066 C GLY 347 61.504 9.069 16.182 1.00 30.72 ATOM 1067 O GLY 60.967 8.160 16.812 1.00 30.89 347 **ATOM** 1068 N VAL 348 62.051 10.132 16.765 1.00 31.30 **ATOM** 1069 CA VAL 348 62.084 10.291 18.221 1.00 31.27 **ATOM** 1070 CB VAL 348 62.843 11.612 18.620 1.00 31.66 **ATOM** 1071 CG1 VAL 348 62.071 12.841 18.146 1.00 20.19 **ATOM** 1072 CG2 VAL 348 63.080 11.651 20.118 1.00 24.77 **ATOM** 1073 C VAL 348 60.683 10.273 18.855 1.00 33.84 VAL **ATOM** 1074 O 348 60.546 10.034 20.050 1.00 29.99 **ATOM** 1075 N VAL 349 59.649 10.518 18.049 1.00 33.31 **ATOM** 1076 CA VAL 349 58.270 10.495 18.538 1.00 32.23 **ATOM** 1077 CB VAL 349 57.279 10.911 17.415 1.00 32.59 **ATOM** 1078 CG1 VAL 349 55.837 10.678 17.838 1.00 33.68 **ATOM** 1079 CG2 VAL 349 57.474 12.378 17.103 1.00 32.30 ATOM 1080 C VAL 349 57.931 9.094 19.050 1.00 34.91 ATOM 1081 O VAL 349 57.133 8.932 19.980 1.00 33.73 **ATOM** 1082 N SER 350 58.551 8.081 18.444 1.00 32.81 ATOM 1083 CA SER 350 58.335 6.704 18.853 1.00 30.10 **ATOM** 1084 CB SER 350 59.041 5.746 17.904 1.00 24.95 **ATOM** 1085 OG SER 350 58.943 4.417 18.387 1.00 23.16 **ATOM** 1086 C SER 350 58.863 6.486 20.266 1.00 31.59 **ATOM** 1087 O SER 350 58.207 5.845 21.086 1.00 37.62 **ATOM** 1088 N **ASP** 351 60.055 7.007 20.546 1.00 28.60

ATOM 1089 CA ASP 351 60.652 6.863 21.867 1.00 29.82 ATOM 1090 CB ASP 351 62.048 7.491 21.919 1.00 27.49 ATOM 1091 CG ASP 351 63.030 6.806 21.000 1.00 30.22 **ATOM** 1092 OD1 ASP 351 63.411 7.412 19.974 1.00 32.61 ATOM 1093 OD2 ASP 351 63.422 5.661 21.301 1.00 30.02 ATOM 1094 C₋ ASP 351 59.785 7.548 22.913 1.00 30.63 ATOM 1095 O ASP 351 59.632 7.055 24.027 1.00 29.54 ATOM 1096 N ALA 352 59.222 8.692 22.537 1.00 25.33 1097 CA ALA 352 ATOM 58.390 9.464 23.432 1.00 28.59 ATOM 1098 CB ALA 352 58.011 10.798 22.788 1.00 20.95 **ATOM** 1099 C ALA 352 57.136 8.695 23.831 1.00 29.69 ATOM 1100 O ALA 352 56.711 8.753 24.982 1.00 30.36 **ATOM** 1101 N ILE 353 56.557 7.979 22.876 1.00 27.63 1102 CA ILE 353 55.345 7.227 23.129 1.00 27.55 ATOM **ATOM** 1103 CB ILE 353 54.611 6.925 21.805 1.00 28.04 **ATOM** 1104 CG2 ILE 353 53.329 6.111 22.065 1.00 23.68 **ATOM** 1105 CG1 ILE 353 54.269 8.251 21.119 1.00 27.33 1106 CD1 ILE 353 **ATOM** 53.637 8.105 19.734 1.00 26.23 1107 C ILE 353 ATOM 55.631 5.943 23.901 1.00 30.88 **ATOM** 1108 O ILE 353 54.880 5.597 24.814 1.00 31.22 ATOM 1109 N PHE 354 56.710 5.240 23.549 1.00 29.86 ATOM 1110 CA PHE 354 57.056 4.022 24.275 1.00 31.08 ATOM 1111 CB PHE 354 58.227 3.274 23.619 1.00 28.80 1112 CG PHE 354 ATOM 57.799 2.322 22.523 1.00 28.80 354 ATOM 1113 CD1 PHE 57.330 2.804 21.292 1.00 30.96 ATOM 1114 CD2 PHE 354 57.811 0.939 22.749 1.00 29.45 **ATOM** 1115 CE1 PHE 354 56.864 1.909 20.281 1.00 27.12 ATOM 1116 CE2 PHE 354 57.354 0.026 21.761 1.00 25.19 **ATOM** 1117 CZ PHE 354 56.879 0.518 20.521 1.00 28.09 **ATOM** 1118 C PHE 354 57.398 4.349 25.721 1.00 29.17 ATOM 1119 O PHE 354 57.001 3.625 26.631 1.00 32.62 **ATOM** 1120 N ASP 355 58.133 5.438 25.925 1.00 23.86 **ATOM** 1121 CA ASP 355 58.508 5.873 27.262 1.00 25.34 **ATOM** 1122 CB ASP 355 59.434 7.083 27.180 1.00 21.41 **ATOM** 1123 CG ASP 355 60.846 6.708 26.769 1.00 32.08 **ATOM** 1124 OD1 ASP 355 61.051 5.595 26.226 1.00 33.58 ATOM 1125 OD2 ASP 355 61.756 7.534 26.970 1.00 33.20 ATOM 1126 C ASP 355 57.254 6.211 28.062 1.00 27.86 **ATOM** 1127 O ASP 355 57.167 5.916 29.252 1.00 32.42 ATOM 1128 N LEU 356 56.276 6.821 27.401 1.00 26.84 1129 CA LEU 356 ATOM 55.031 7.164 28.066 1.00 28.66 **ATOM** 1130 CB LEU 356 54.112 7.953 27.131 1.00 25.37 **ATOM** 1131 CG LEU 356 52.787 8.427 27.742 1.00 27.61 1132 CD1 LEU 356 ATOM 53.056 9.452 28.842 1.00 25.43 **ATOM** 1133 CD2 LEU 356 51.924 9.057 26.667 1.00 27.49 ATOM 1134 C LEU 356 54.334 5.875 28.473 1.00 30.44

ATOM 1135 O LEU 356 53.873 5.743 29.601 1.00 31.55 1136 N ATOM GLY 357 54.266 4.928 27.536 1.00 32.69 1137 CA GLY **ATOM** 357 53.621 3.652 27.787 1.00 29.87 **ATOM** 1138 C GLY 357 2.884 28.939 1.00 33.12 54.239 **ATOM** 1139 O **GLY** 357 53.524 2.268 29.732 1.00 29.41 1140 N. MET **ATOM** 358 2.911 29.026 1.00 33.31 55.570 **ATOM** 1141 CA MET 358 56.277 2.217 30.100 1.00 35.87 1142 CB MET **ATOM** 2.265 29.871 1.00 34.56 358 57.794 **ATOM** 1143 CG MET 358 58.265 1.608 28.576 1.00 46.43 **ATOM** 1144 SD MET 358 60.073 1.600 28.351 1.00 42.13 **ATOM** 1145 CE MET 358 60.429 3.306 28.411 1.00 44.29 **ATOM** 1146 C **MET** 358 55.948 2.884 31.434 1.00 33.26 **MET** ATOM 1147 O 358 55.802 2.222 32.453 1.00 36.39 **ATOM** 1148 N SER 359 55.825 4.202 31.398 1.00 33.31 **ATOM** 1149 CA SER 359 55.533 4.998 32.580 1.00 34.39 1150 CB SER **ATOM** 359 55.859 6.463 32.303 1.00 30.84 **ATOM** 1151 OG SER 359 55.487 7.265 33.404 1.00 47.14 **ATOM** 1152 C SER 359 54.094 4.897 33.072 1.00 36.43 **ATOM** 1153 O SER 359 53.833 5.073 34.260 1.00 35.46 1154 N LEU ATOM 360 53.165 4.617 32.156 1.00 36.74 1155 CA LEU **ATOM** 360 51.750 4.519 32.493 1.00 35.44 **ATOM** 1156 CB LEU 360 50.889 4.817 31.263 1.00 34.16 1157 CG LEU **ATOM** 360 50.896 6.263 30.751 1.00 34.59 **ATOM** 1158 CD1 LEU 360 50.031 6.353 29.513 1.00 33.53 **ATOM** 1159 CD2 LEU 360 50.376 7.211 31.836 1.00 31.69 **ATOM** 1160 C LEU 360 51.324 3.192 33.088 1.00 38.72 **ATOM** 1161 O LEU 360 50.185 3.058 33.546 1.00 38.29 SER **ATOM** 1162 N 361 52.227 2.214 33.080 1.00 40.96 **ATOM** 1163 CA SER 361 51.938 0.897 33.636 1.00 45.67 **ATOM** 1164 CB SER 361 53.131 -0.044 33.436 1.00 46.45 **ATOM** 1165 OG SER 361 53.362 -0.296 32.061 1.00 51.81 **ATOM** 1166 C SER 361 51.628 1.004 35.124 1.00 44.49 361 **ATOM** 1167 O SER 50.724 0.337 35.630 1.00 46.67 **ATOM** 1168 N SER 362 52.385 1.858 35.809 1.00 41.44 1169 CA SER **ATOM** 362 52.231 2.081 37.245 1.00 42.13 **ATOM** 1170 CB SER 362 53.431 2.876 37.779 1.00 42.61 ATOM 1171 OG SER 362 54.647 2.215 37.492 1.00 51.87 **ATOM** 1172 C SER 362 50.951 2.832 37.610 1.00 38.41 **ATOM** 1173 O **SER** 362 50.444 2.700 38.722 1.00 38.01 **ATOM** 1174 N PHE 363 50.443 3.631 36.672 1.00 34.55 **ATOM** 1175 CA PHE 363 49.232 4.404 36.906 1.00 32.96 49.109 **ATOM** 1176 CB PHE 363 5.518 35.859 1.00 31.99 **ATOM** 1177 CG PHE 363 50.093 6.659 36.058 1.00 29.97 **ATOM** 1178 CD1 PHE 363 49.667 7.872 36.594 1.00 30.61 363 **ATOM** 1179 CD2 PHE 51.445 6.501 35.731 1.00 32.02 50.579 8.940 36.803 1.00 33.67 363 ATOM 1180 CE1 PHE

ATOM 1181 CE2 PHE 363 52.376 7.552 35.934 1.00 30.91 1182 CZ PHE **ATOM** 363 51.938 8.777 36.473 1.00 29.33 **ATOM** 1183 C PHE 363 47.973 3.554 36.916 1.00 30.52 **ATOM** 1184 O PHE 363 46.971 3.947 37.491 1.00 32.19 **ATOM** 1185 N ASN 364 48.036 2.384 36.283 1.00 33.51 1186 CA ASN ATOM 364 46.894 1.471 36.216 1.00 38.03 **ATOM** 1187 CB ASN 46.754 0.711 37.539 1.00 42.32 364 ATOM 1188 CG ASN 364 47.824 -0.361 37.713 1.00 53.11 ATOM 1189 OD1 ASN 364 47.815 -1.370 37.012 1.00 59.51 ATOM 1190 ND2 ASN 48.751 -0.138 38.639 1.00 55.95 364 ATOM 1191 C ASN 45.574 2.161 35.871 1.00 31.89 364 ATOM 1192 O ASN 364 44.587 2.027 36.588 1.00 30.28 **ATOM** 1193 N LEU 365 45.561 2.883 34.751 1.00 27.62 **ATOM** 1194 CA LEU 365 44.365 3.606 34.317 1.00 29.36 1195 CB LEU ATOM 365 44.738 4.627 33.240 1.00 27.54 **ATOM** 1196 CG LEU 365 45.826 5.659 33.576 1.00 38.91 **ATOM** 1197 CD1 LEU 365 46.115 6.499 32.338 1.00 34.47 1198 CD2 LEU 365 ATOM 45.394 6.546 34.743 1.00 34.24 ATOM 1199 C LEU 365 43.264 2.691 33.774 1.00 26.23 **ATOM** 1200 O LEU 365 43.546 1.648 33.197 1.00 27.06 **ATOM** 1201 N ASP 366 42.011 3.074 33.991 1.00 25.23 1202 CA ASP ATOM 366 40.892 2.307 33.462 1.00 26.07 **ATOM** 1203 CB ASP 366 39.832 2.008 34.538 1.00 29.68 **ATOM** 1204 CG ASP 366 39.337 3.253 35.261 1.00 35.74 **ATOM** 1205 OD1 ASP 366 39.438 4.371 34.717 1.00 36.78 ATOM 1206 OD2 ASP 366 38.803 3.100 36.378 1.00 41.23 **ATOM** 1207 C ASP 366 40.274 3.100 32.305 1.00 27.70 ATOM 1208 O **ASP** 366 40.748 4.191 31.975 1.00 31.94 **ATOM** 1209 N ASP 367 39.223 2.564 31.693 1.00 29.18 **ATOM** 1210 CA ASP 367 38.594 3.233 30.560 1.00 32.72 **ATOM** 1211 CB ASP 367 37.428 2.395 30.018 1.00 38.04 **ATOM** 1212 CG ASP 367 37.855 0.995 29.606 1.00.42.43 **ATOM** 1213 OD1 ASP 367 38.913 0.852 28.956 1.00 35.95 **ATOM** 1214 OD2 ASP 367 37.115 0.034 29.917 1.00 51.42 **ATOM** 1215 C ASP 367 38.093 4.631 30.881 1.00 33.71 38.059 5.506 30.013 1.00 38.30 **ATOM** 1216 O ASP 367 **ATOM** 1217 N THR 368 37.705 4.852 32.132 1.00 31.06 **ATOM** 1218 CA THR 368 37.199 6.155 32.543 1.00 26.28 1219 CB THR 368 **ATOM** 36.537 6.066 33.922 1.00 27.30 **ATOM** 1220 OG1 THR 368 35.461 5.127 33.861 1.00 33.42 **ATOM** 1221 CG2 THR 368 36.003 7.423 34.355 1.00 25.16 **ATOM** 1222 C THR 368 38.303 7.194 32.593 1.00 21.13 **ATOM** 1223 O THR 368 38.133 8.314 32.104 1.00 23.17 1224 N GLU **ATOM** 369 39.431 6.816 33.179 1.00 21.32 **ATOM** 1225 CA GLU 369 40.565 7.720 33.317 1.00 28.00 1226 CB GLU 369 ATOM 41.582 7.107 34.277 1.00 32.79

ATOM 1227 CG GLU 40.944 369 6.804 35.619 1.00 36.29 **ATOM** 1228 CD GLU 369 41.834 6.026 36.546 1.00 41.03 **ATOM** 1229 OE1 GLU 369 42.361 4.967 36.123 1.00 42.05 1230 OE2 GLU **ATOM** 369 41.986 6.458 37.705 1.00 42.03 **ATOM** 1231 C GLU 369 41.201 8.047 31.970 1.00 25.57 **ATOM** 1232 O-GLU 369 41.626 9.175 31.741 1.00 20.56 **ATOM** 1233 N VAL 370 41.249 7.055 31.080 1.00 25.39 ATOM 1234 CA VAL 370 41.794 7.278 29.745 1.00 25.99 ATOM 1235 CB VAL 370 5.936 28.977 1.00 26.15 42.005 ATOM 1236 CG1 VAL 42.450 6.216 27.539 1.00 27.65 370 ATOM 1237 CG2 VAL 370 43.056 5.086 29.685 1.00 17.70 **ATOM** 1238 C VAL 370 40.814 8.164 28.966 1.00 26.49 ATOM 1239 O VAL 41.226 9.038 28.202 1.00 28.16 370 **ATOM** 1240 N ALA 371 39.514 7.950 29.184 1.00 21.01 **ATOM** 1241 CA ALA 371 38.486 8.730 28.510 1.00 19.57 ATOM 1242 CB ALA 371 37.116 8.136 28.783 1.00 18.62 **ATOM** 1243 C ALA 371 38.512 10.191 28.947 1.00 23.48 ATOM 1244 O ALA 371 38.500 11.103 28.111 1.00 32.67 **ATOM** 1245 N LEU 372 38.540 10.414 30.256 1.00 22.89 1246 CA LEU ATOM 372 38.560 11.772 30.806 1.00 23.28 1247 CB LEU **ATOM** 372 38.517 11.709 32.343 1.00 27.76 **ATOM** 1248 CG LEU 372 37.155 11.306 32.924 1.00 21.18 **ATOM** 1249 CD1 LEU 372 37.289 10.891 34.381 1.00 27.64 ATOM 1250 CD2 LEU 36.197 12.480 32.763 1.00 20.90 372 **ATOM** 1251 C LEU 372 39.804 12.505 30.357 1.00 21.34 ATOM 1252 O LEU 372 39.779 13.708 30.086 1.00 23.16 ATOM 1253 N LEU 373 40.896 11.761 30.276 1.00 24.42 **ATOM** 1254 CA LEU 373 42.177 12.302 29.855 1.00 23.78 ATOM 1255 CB LEU 373 43.222 11.205 30.007 1.00 22.18 **ATOM** 1256 CG LEU 373 44.724 11.456 30.036 1.00 31.52 **ATOM** 1257 CD1 LEU 373 45.099 12.565 31.001 1.00 31.93 **ATOM** 1258 CD2 LEU 373 45.382 10.152 30.460 1.00 30.24 **ATOM** 1259 C LEU 373 42.025 12.757 28.399 1.00 25.69 **ATOM** 1260 O LEU 373 42.469 13.842 28.025 1.00 30.13 **ATOM** 1261 N GLN 374 41.370 11.934 27.587 1.00 26.24 **ATOM** 1262 CA GLN 374 41.151 12.269 26.184 1.00 21.60 ATOM 1263 CB GLN 374 40.501 11.091 25.444 1.00 24.57 **ATOM** 1264 CG GLN 374 41.428 9.900 25.234 1.00 21.02 **ATOM** 1265 CD GLN 374 40.762 8.744 24.501 1.00 22.86 **ATOM** 1266 OE1 GLN 374 41.407 7.754 24.174 1.00 24.07 **ATOM** 1267 NE2 GLN 374 39.466 8.865 24.249 1.00 25.59 **ATOM** 1268 C GLN 374 40.267 13.498 26.070 1.00 20.66 **ATOM** 1269 O GLN 374 40.518 14.366 25.242 1.00 24.47 1270 N ALA **ATOM** 375 39.237 13.579 26.902 1.00 16.26 1271 CA ALA **ATOM** 375 38.337 14.727 26.870 1.00 17.16 ATOM 1272 CB ALA 375 37.156 14.491 27.803 1.00 19.53

ATOM 1273 C ALA 375 39.056 16.024 27.252 1.00 25.13 1274 O **ATOM** ALA 375 38.722 17.100 26.750 1.00 23.81 1275 N **ATOM VAL** 376 40.036 15.926 28.156 1.00 24.57 **ATOM** 1276 CA VAL 376 40.796 17.101 28.568 1.00 25.80 **ATOM** 1277 CB VAL 376 41.711 16.792 29.814 1.00 26.48 ATOM 1278 CG1 VAL 376 42.625 17.971 30.102 1.00 23.20 ATOM 1279 CG2 VAL 376 40.845 16.521 31.044 1.00 19.08 ATOM 1280 C VAL 376 41.653 17.580 27.396 1.00 25.69 ATOM 1281 O VAL 376 41.775 18.780 27.151 1.00 27.87 ATOM 1282 N LEU 377 42.249 16.637 26.666 1.00 23.09 **ATOM** 1283 CA LEU 377 43.071 16.982 25.513 1.00 22.86 **ATOM** 1284 CB LEU 377 43.748 15.730 24.962 1.00 18.50 **ATOM** 1285 CG LEU 377 44.814 15.096 25.867 1.00 22.65 **ATOM** 1286 CD1 LEU 377 45.144 13.708 25.374 1.00 16.70 1287 CD2 LEU 377 **ATOM** 46.070 15.987 25.901 1.00 19.58 **ATOM** 1288 C LEU 377 42.197 17.634 24.430 1.00 26.14 **ATOM** 1289 O LEU 377 42.579 18.638 23.830 1.00 20.62 **ATOM** 1290 N LEU 378 41.016 17.057 24.208 1.00 28.99 ATOM 1291 CA LEU 378 40.076 17.578 23.218 1.00 28.87 ATOM 1292 CB LEU 378 38.814 16.710 23.182 1.00 26.89 **ATOM** 1293 CG LEU 378 37.637 17.167 22.311 1.00 28.83 **ATOM** 1294 CD1 LEU 378 38.053 17.273 20.840 1.00 27.97 **ATOM** 1295 CD2 LEU 378 36.496 16.175 22.478 1.00 27.69 **ATOM** 1296 C LEU 378 39.693 19.025 23.504 1.00 31.09 **ATOM** 1297 O LEU 378 39.812 19.883 22.629 1.00 31.77 **ATOM** 1298 N MET 379 39.247 19.297 24.729 1.00 31.44 **ATOM** 1299 CA MET 379 38.841 20.649 25.104 1.00 32.62 **ATOM** 37.876 20.603 26.293 1.00 31.45 1300 CB MET 379 **ATOM** 1301 CG MET 379 36.586 19.855 26.010 1.00 38.75 1302 SD MET **ATOM** 379 35.646 20.541 24.601 1.00 41.27 **ATOM** 1303 CE MET 379 34.231 19.443 24.609 1.00 35.68 ATOM 1304 C MET 379 39.980 21.613 25.421 1.00 33.72 **ATOM** 1305 O **MET** 379 39.940 22.297 26.446 1.00 36.29 1306 N 40.981 21.676 24.543 1.00 34.49 **ATOM** SER 380 ATOM 1307 CA SER 380 42.116 22.585 24.721 1.00 33.97 **ATOM** 1308 CB SER 380 43.371 22.025 24.061 1.00 31.24 1309 OG SER 380 ATOM 43.771 20.814 24.674 1.00 39.42 **ATOM** 1310 C SER 380 41.772 23.926 24.088 1.00 39.69 **ATOM** 1311 O SER 380 41.787 24.069 22.864 1.00 44.64 **ATOM** 1312 N SER 381 41.472 24.907 24.927 1.00 41.04 ATOM 1313 CA SER 381 41.090 26.234 24.462 1.00 44.91 **ATOM** 1314 CB SER 381 40.406 27.004 25.594 1.00 44.50 **ATOM** 1315 OG SER 381 41.294 27.177 26.678 1.00 45.42 ATOM 1316 C SER 381 42.231 27.084 23.921 1.00 44.59 SER 42.012 28.227 23.516 1.00 49.32 **ATOM** 1317 O 381 **ATOM ASP** 43.440 26.541 23.896 1.00 43.75 1318 N 382

ATOM	1319 CA ASP 382	44.571 27.315 23.407 1.00 43.93
ATOM	1 1320 CB ASP 382	45.817 27.047 24.257 1.00 48.39
ATOM	1321 CG ASP 382	46.319 25.632 24.113 1.00 53.23
ATOM	1322 OD1 ASP 382	45.590 24.702 24.517 1.00 56.97
ATOM	1323 OD2 ASP 382	47.440 25.449 23.584 1.00 58.91
ATOM		44.900 27.026 21.955 1.00 41.09
ATOM	1325 O ASP 382	45.912 27.502 21.446 1.00 40.93
ATOM	1326 N ARG 383	44.068 26.236 21.287 1.00 42.63
ATOM	1327 CA ARG 383	44.316 25.937 19.876 1.00 43.32
ATOM	1328 CB ARG 383	43.289 24.935 19.331 1.00 42.31
ATOM	1329 CG ARG 383	43.174 23.619 20.095 1.00 40.83
ATOM	1330 CD ARG 383	44.478 22.835 20.139 1.00 38.09
ATOM	1331 NE ARG 383	44.271 21.542 20.787 1.00 37.33
ATOM		45.235 20.690 21.115 1.00 38.35
ATOM	1333 NH1 ARG 383	46.505 20.972 20.850 1.00 33.70
ATOM	1334 NH2 ARG 383	44.922 19.545 21.704 1.00 35.46
ATOM	1335 C ARG 383	44.166 27.256 19.127 1.00 44.96
ATOM	1336 O ARG 383	43.214 28.006 19.361 1.00 45.60
ATOM	1337 N PRO 384	45.112 27.574 18.230 1.00 45.33
ATOM	1338 CD PRO 384	46.330 26.852 17.836 1.00 46.85
ATOM	1339 CA PRO 384	45.024 28.830 17.484 1.00 47.37
ATOM	1340 CB PRO 384	46.323 28.823 16.672 1.00 46.90
ATOM	1341 CG PRO 384	47.257 27.998 17.552 1.00 46.41
ATOM	1342 C PRO 384	43.788 28.910 16.590 1.00 48.29
ATOM	1343 O PRO 384	43.394 27.927 15.960 1.00 48.34
ATOM	1344 N GLY 385	43.176 30.090 16.552 1.00 49.88
ATOM	1345 CA GLY 385	42.013 30.290 15.712 1.00 50.35
ATOM	1346 C GLY 385	40.669 29.958 16.324 1.00 50.70
ATOM ATOM	1347 O GLY 385	39.639 30.201 15.697 1.00 53.48
ATOM	1348 N LEU 386	40.663 29.404 17.529 1.00 49.04
ATOM	1349 CA LEU 386 1350 CB LEU 386	39.405 29.057 18.182 1.00 50.53
ATOM	1351 CG LEU 386	39.655 28.433 19.558 1.00 45.17
ATOM	1352 CD1 LEU 386	40.245 27.019 19.544 1.00 48.26 40.502 26.564 20.970 1.00 41.68
ATOM	1353 CD2 LEU 386	39.285 26.065 18.836 1.00 38.40
ATOM	1354 C LEU 386	38.495 30.268 18.319 1.00 52.13
ATOM	1355 O LEU 386	38.955 31.395 18.476 1.00 53.67
ATOM	1356 N ALA 387	37.193 30.020 18.261 1.00 53.42
ATOM	1357 CA ALA 387	36.225 31.093 18.354 1.00 56.01
ATOM	1358 CB ALA 387	35.221 30.976 17.202 1.00 56.47
ATOM	1359 C ALA 387	35.482 31.144 19.681 1.00 55.52
ATOM	1360 O ALA 387	35.491 32.171 20.358 1.00 53.75
ATOM	1361 N CYS 388	34.854 30.038 20.065 1.00 56.03
ATOM	1362 CA CYS 388	34.072 30.036 21.312 1.00 59.57
ATOM	1363 CB CYS 388	32.724 29.351 21.089 1.00 59.23
ATOM	1364 SG CYS 388	31.314 30.363 21.641 1.00 58.64
		2.02. 20.202 21.071 1.00 20.07

ATOM 1365 C CYS 34.846 29.289 22.398 1.00 62.18 388 ATOM 1366 O **CYS** 388 34.458 28.190 22.790 1.00 67.88 **ATOM** 1367 N VAL 389 35.955 29.950 22.760 1.00 60.78 **ATOM** 1368 CA VAL 389 37.005 29.583 23.713 1.00 57.70 **ATOM** 1369 CB VAL 389 38.202 30.580 23.565 1.00 57.09 ATOM 1370 CG1 VAL 389 39.351 30.194 24.494 1.00 59.03 **ATOM** 1371 CG2 VAL 389 38.671 30.618 22.124 1.00 53.98 ATOM 36.661 29.515 25.195 1.00 57.77 1372 C VAL 389 **ATOM** 1373 O VAL 36.943 28.513 25.851 1.00 60.94 389 ATOM 1374 N GLU 390 36.102 30.594 25.732 1.00 52.68 **ATOM** 1375 CA GLU 390 35.738 30.636 27.138 1.00 48.41 **ATOM** 1376 CB GLU 390 35.001 31.928 27.451 1.00 45.19 **ATOM** 1377 C GLU 390 34.868 29.439 27.459 1.00 47.63 **ATOM** 1378 O GLU 390 34.986 28.837 28.529 1.00 51.95 ATOM 1379 N ARG 391 34.002 29.082 26.517 1.00 47.11 **ATOM** 1380 CA ARG 391 33.099 27.950 26.699 1.00 51.64 ATOM 1381 CB ARG 391 32.050 27.930 25.588 1.00 54.22 ATOM 1382 CG ARG 391 30.830 27.094 25.915 1.00 64.20 **ATOM** 1383 CD ARG 391 29.867 27.074 24.748 1.00 73.80 **ATOM** 1384 NE ARG 391 28.533 26.622 25.128 1.00 79.76 1385 CZ ARG 27.714 27.298 25.929 1.00 84.27 ATOM 391 **ATOM** 1386 NH1 ARG 391 28.090 28.465 26.439 1.00 85.28 ATOM 1387 NH2 ARG 391 26.515 26.809 26.217 1.00 86.84 ATOM 1388 C ARG 391 33.890 26.644 26.684 1.00 48.18 **ATOM** 1389 O ARG 391 33.504 25.671 27.330 1.00 49.57 **ATOM** 1390 N ILE 392 34.987 26.625 25.936 1.00 45.01 1391 CA ILE **ATOM** 392 35.835 25.440 25.858 1.00 48.77 **ATOM** 1392 CB ILE 36.854 25.565 24.692 1.00 46.45 392 **ATOM** 1393 CG2 ILE 392 37.798 24.370 24.679 1.00 42.35 **ATOM** 1394 CG1 ILE 392 36.086 25.664 23.367 1.00 49.69 1395 CD1 ILE ATOM 392 36.950 25.897 22.136 1.00 51.09 ATOM 1396 C ILE 392 36.570 25.246 27.192 1.00 50.90 **ATOM** 1397 O ILE 392 36.731 24.118 27.657 1.00 52.21 **ATOM** 1398 N GLU 393 36.999 26.346 27.811 1.00 50.43 ATOM 1399 CA GLU 393 37.673 26.267 29.101 1.00 50.30 **ATOM** 1400 CB GLU 393 38.202 27.638 29.531 1.00 53.97 ATOM 1401 CG GLU 393 39.322 28.168 28.658 1.00 62.18 **ATOM** 1402 CD GLU 393 39.911 29.478 29.168 1.00 67.69 **ATOM** 1403 OE1 GLU 393 40.869 29.977 28.537 1.00 66.42 **ATOM** 1404 OE2 GLU 393 39.423 30.009 30.191 1.00 70.64 36.686 25.765 30.145 1.00 49.31 ATOM 1405 C GLU 393 **ATOM** 1406 O GLU 393 37.018 24.923 30.980 1.00 49.53 **ATOM** 1407 N LYS 394 35.468 26.286 30.090 1.00 46.07 **ATOM** 1408 CA LYS 394 34.428 25.893 31.022 1.00 45.76 **ATOM** 1409 CB LYS 394 33.147 26.666 30.727 1.00 43.85 **ATOM** 1410 C LYS 394 34.188 24.391 30.909 1.00 46.69

1411 O ATOM LYS 394 33.982 23.699 31.911 1.00 49.13 **ATOM** 1412 N TYR 395 34.223 23.887 29.679 1.00 46.57 1413 CA TYR 395 **ATOM** 34.014 22.467 29.427 1.00 43.33 **ATOM** 1414 CB TYR 395 33.818 22.211 27.929 1.00 48.44 ATOM 1415 CG TYR 395 32.493 22.710 27.335 1.00 53.83 1416 CD1 TYR 395 **ATOM** 32.302 22.727 25.947 1.00 56.43 **ATOM** 1417 CE1 TYR 395 31.078 23.148 25.374 1.00 59.73 ATOM 1418 CD2 TYR 395 31.434 23.132 28.153 1.00 56.47 ATOM 1419 CE2 TYR 395 30.198 23.559 27.592 1.00 62.60 1420 CZ TYR 395 ATOM 30.037 23.562 26.200 1.00 63.18 **ATOM** 1421 OH TYR 395 28.834 23.962 25.635 1.00 64.46 1422 C ATOM TYR 395 35.189 21.635 29.938 1.00 37.30 **ATOM** 1423 O TYR 395 34.993 20.599 30.564 1.00 34.10 **ATOM** 1424 N GLN 396 36.408 22.091 29.671 1.00 31.92 **ATOM** 1425 CA GLN 396 37.584 21.363 30.120 1.00 34.81 **ATOM** 1426 CB GLN 396 38.861 21.987 29.560 1.00 32.64 **ATOM** 1427 CG GLN 396 40.114 21.183 29.882 1.00 29.57 **ATOM** 1428 CD GLN 396 41.370 21.827 29.352 1.00 29.46 1429 OE1 GLN 41.648 22.982 29.649 1.00 34.65 ATOM 396 **ATOM** 1430 NE2 GLN 396 42.139 21.088 28.570 1.00 27.21 37.647 21.342 31.647 1.00 37.13 **ATOM** 1431 C GLN 396 ATOM 1432 O GLN 396 37.939 20.302 32.236 1.00 37.36 **ATOM** 1433 N ASP 37.371 22.484 32.284 1.00 38.61 397 **ATOM** 1434 CA ASP 397 37.393 22.555 33.742 1.00 40.37 ATOM 1435 CB ASP 397 37.099 23.973 34.240 1.00 40.51 **ATOM** 1436 CG ASP 397 38.130 24.974 33.772 1.00 43.77 **ATOM** 1437 OD1 ASP 397 39.330 24.632 33.775 1.00 46.50 **ATOM** 1438 OD2 ASP 397 37.750 26.109 33.422 1.00 51.34 **ATOM** 1439 C ASP 397 36.352 21.601 34.295 1.00 38.62 **ASP ATOM** 1440 O 397 36.515 21.034 35.372 1.00 39.20 **ATOM** 1441 N SER 398 35.282 21.423 33.540 1.00 37.84 **ATOM** 1442 CA SER 398 34.221 20.524 33.942 1.00 37.80 **ATOM** 1443 CB SER 398 33.039 20.669 32.984 1.00 34.28 **ATOM** 1444 OG SER 398 31.981 19.815 33.360 1.00 46.60 **ATOM** 1445 C SER 398 34.752 19.082 33,939 1.00 38.41 **ATOM** 1446 O SER 34.372 18.274 34.787 1.00 39.98 398 ATOM 1447 N PHE 399 35.630 18.772 32.987 1.00 34.82 **ATOM** 1448 CA PHE 399 36.213 17.433 32.885 1.00 35.96 1449 CB PHE ATOM 399 36.809 17.181 31.493 1.00 35.75 **ATOM** 1450 CG PHE 399 35.775 16.936 30.419 1.00 39.30 **ATOM** 1451 CD1 PHE 399 35.640 17.826 29.344 1.00 39.86 **ATOM** 1452 CD2 PHE 399 34.936 15.819 30.487 1.00 36.81 **ATOM** 1453 CE1 PHE 399 34.674 17.607 28.330 1.00 41.25 399 **ATOM** 1454 CE2 PHE 33.962 15.577 29.488 1.00 43.61 **ATOM** 1455 CZ PHE 399 33.829 16.480 28.402 1.00 40.34 ATOM 1456 C PHE 399 37.306 17.217 33.921 1.00 33.48

ATOM 1457 O PHE 399 37.406 16.139 34.512 1.00 26.86 **ATOM** 1458 N LEU 400 38.132 18.239 34.118 1.00 31.47 **ATOM** 1459 CA LEU 400 39.213 18.162 35.086 1.00 37.41 **ATOM** 1460 CB LEU 400 40.051 19.441 35.038 1.00 34.24 **ATOM** 1461 CG LEU 400 40.934 19.574 33.788 1.00 35.10 1462 CD1 LEU **ATOM** 400 41.469 20.991 33.651 1.00 26.60 **ATOM** 1463 CD2 LEU 400 42.077 18.569 33.884 1.00 29.44 **ATOM** 1464 C LEU 400 38.666 17.931 36.491 1.00 38.84 **ATOM** 1465 O LEU 400 39.137 17.049 37.205 1.00 40.38 **ATOM** 1466 N LEU 401 37.654 18.703 36.870 1.00 42.79 **ATOM** 1467 CA LEU 401 37.056 18.584 38.197 1.00 43.48 1468 CB LEU **ATOM** 401 35.997 19.675 38.406 1.00 44.73 **ATOM** 1469 CG LEU 401 35.322 19.737 39.779 1.00 51.39 **ATOM** 1470 CD1 LEU 401 36.359 20.002 40.866 1.00 50.11 1471 CD2 LEU **ATOM** 401 34.273 20.834 39.778 1.00 49.30 ATOM 1472 C LEU 401 36.433 17.215 38.409 1.00 41.62 **ATOM** 1473 O LEU 401 36.563 16.622 39.482 1.00 45.14 **ATOM** 1474 N ALA 402 35.744 16.712 37.389 1.00 37.92 **ATOM** 1475 CA ALA 402 35.115 15.402 37.484 1.00 29.90 **ATOM** 1476 CB ALA 402 34.196 15.187 36.297 1.00 30.70 **ATOM** 1477 C ALA 402 36.203 14.336 37.508 1.00 28.88 **ATOM** 1478 O ALA 402 36.083 13.322 38.188 1.00 32.14 1479 N PHE 403 **ATOM** 37.274 14.588 36.764 1.00 31.07 **ATOM** 1480 CA PHE 403 38.402 13.656 36.661 1.00 29.90 **ATOM** 1481 CB PHE 403 39.396 14.178 35.605 1.00 27.03 40.434 13.146 35.140 1.00 26.97 ATOM 1482 CG PHE 403 **ATOM** 1483 CD1 PHE 403 41.362 13.509 34.149 1.00 25.55 **ATOM** 1484 CD2 PHE 403 40.475 11.841 35.664 1.00 19.75 42.331 12.588 33.679 1.00 27.90 **ATOM** 1485 CE1 PHE 403 1486 CE2 PHE 403 **ATOM** 41.441 10.899 35.206 1.00 22.56 1487 CZ PHE 403 **ATOM** 42.371 11.273 34.210 1.00 22.24 **ATOM** 1488 C PHE 403 39.081 13.523 38.023 1.00 28.82 1489 O PHE 403 **ATOM** 39.313 12.413 38.495 1.00 26.00 **ATOM** 1490 N GLU 404 39.405 14.652 38.652 1.00 30.25 **ATOM** 1491 CA GLU 404 40.039 14.627 39.966 1.00 34.03 **ATOM** 1492 CB GLU 404 40.264 16.046 40.497 1.00 39.45 **ATOM** 1493 CG GLU 404 40.987 16.076 41.839 1.00 47.68 404 **ATOM** 1494 CD GLU 41.062 17.465 42.446 1.00 54.02 1495 OE1 GLU 404 **ATOM** 41.607 18.380 41.796 1.00 57.27 404 **ATOM** 1496 OE2 GLU 40.573 17.638 43.585 1.00 63.85 404 39.164 13.860 40.960 1.00 36.01 **ATOM** 1497 C GLU 1498 O GLU 404 **ATOM** 39.661 12.997 41.701 1.00 38.64 1499 N HIS **ATOM** 405 37.870 14.168 40.975 1.00 29.56 ATOM 1500 CA HIS 405 36.949 13.508 41.892 1.00 31.69 405 **ATOM** 1501 CB HIS 35.534 14.077 41.757 1.00 33.75 1502 CG HIS 405 35.401 15.498 42.213 1.00 34.75 ATOM

ATOM 1503 CD2 HIS 405 36.308 16.361 42.730 1.00 34.58 **ATOM** 1504 ND1 HIS 405 34.207 16.187 42.146 1.00 32.43 **ATOM** 1505 CE1 HIS 405 34.385 17.414 42.598 1.00 36.15 **ATOM** 1506 NE2 HIS 405 35.650 17.549 42.960 1.00 39.84 **ATOM** 1507 C HIS 405 36.904 12.013 41.673 1.00 34.21 **ATOM** 1508 O- HIS 405 36.700 11.247 42.624 1.00 37.06 ATOM 1509 N TYR 406 37.081 11.594 40.419 1.00 30.83 **ATOM** 1510 CA TYR 406 37.059 10.173 40.093 1.00 28.85 **ATOM** 1511 CB TYR 406 37.018 9.959 38.575 1.00 31.48 ATOM 1512 CG TYR 406 36.879 8.490 38.181 1.00 23.49 ATOM 1513 CD1 TYR 406 35.683 7.798 38.397 1.00 19.42 ATOM 1514 CE1 TYR 406 35.556 6.427 38.059 1.00 23.80 ATOM 1515 CD2 TYR 406 37.950 7.794 37.624 1.00 21.81 1516 CE2 TYR **ATOM** 406 37.838 6.421 37.278 1.00 24.64 ATOM 1517 CZ TYR 406 36.639 5.753 37.503 1.00 21.56 **ATOM** 1518 OH TYR 406 36.537 4.404 37.186 1.00 24.96 ATOM 1519 C **TYR** 406 38.318 9.526 40.638 1.00 24.24 **ATOM** 1520 O TYR 406 38.308 8.375 41.050 1.00 27.08 **ATOM** 1521 N ILE 39.407 10.278 40.617 1.00 25.76 407 **ATOM** 1522 CA ILE 407 40.688 9.799 41.105 1.00 33.75 ATOM 1523 CB ILE 407 41.815 10.822 40.796 1.00 34.23 **ATOM** 1524 CG2 ILE 407 43.121 10.400 41.435 1.00 32.46 **ATOM** 1525 CG1 ILE 41.959 10.972 39.275 1.00 43.30 407 **ATOM** 1526 CD1 ILE 407 42.267 9.677 38.523 1.00 40.40 **ATOM** 1527 C ILE 407 40.620 9.556 42.613 1.00 39.03 **ATOM** 1528 O ILE 41.192 8.583 43.107 1.00 35.18 407 **ATOM** 1529 N ASN 408 39.916 10.440 43.335 1.00 37.25 **ATOM** 1530 CA ASN 408 39.778 10.292 44.777 1.00 37.01 ATOM 1531 CB ASN 408 39.099 11.514 45.400 1.00 32.27 **ATOM** 1532 CG ASN 408 39.887 12.790 45.187 1.00 33.56 **ATOM** 1533 OD1 ASN 408 41.118 12.785 45.225 1.00 31.99 ATOM 1534 ND2 ASN 408 39.182 13.903 44.996 1.00 31.23 **ATOM** 1535 C ASN 408 38.961 9.046 45.055 1.00 38.14 **ATOM** 1536 O ASN 408 39.303 8.243 45.920 1.00 42.16 **ATOM** 1537 N TYR 409 37.874 8.894 44.303 1.00 35.62 **ATOM** 1538 CA TYR 409 37.002 7.733 44.412 1.00 35.91 **ATOM** 1539 CB TYR 409 35.929 7.804 43.323 1.00 34.41 **ATOM** 1540 CG TYR 409 35.196 6.495 43.066 1.00 38.73 **ATOM** 1541 CD1 TYR 409 34.266 5.982 43.980 1.00 41.34 **ATOM** 1542 CE1 TYR 409 33.600 4.745 43.741 1.00 47.16 1543 CD2 TYR **ATOM** 409 35.461 5.752 41.907 1.00 46.20 **ATOM** 1544 CE2 TYR 409 34.814 4.518 41.651 1.00 50.74 **ATOM** 1545 CZ TYR 409 33.891 4.023 42.573 1.00 50.88 1546 OH TYR **ATOM** 409 33.262 2.816 42.302 1.00 53.14 **ATOM** 1547 C TYR 409 37.827 6.459 44.240 1.00 38.16 ATOM 1548 O TYR 409 37.806 5.561 45.082 1.00 41.83

1549 N ARG 410 ATOM 38.551 6.399 43.125 1.00 42.25 1550 CA ARG 410 **ATOM** 39.410 5.272 42.765 1.00 42.83 **ATOM** 1551 CB ARG 410 40.029 5.540 41.392 1.00 36.83 1552 CG ARG 410 ATOM 39.055 5.397 40.249 1.00 34.32 ATOM 1553 CD ARG 410 39.134 3.996 39.681 1.00 36.62 ATOM 1554 NE ARG 410 40.420 3.787 39.013 1.00 38.64 1555 CZ ARG 410 **ATOM** 40.832 2.625 38.517 1.00 35.73 ATOM 1556 NH1 ARG 410 40.068 1.548 38.617 1.00 33.17 1557 NH2 ARG 410 ATOM 42.006 2.544 37.916 1.00 32.70 **ATOM** 1558 C ARG 410 40.520 5.039 43.780 1.00 46.67 **ATOM** 1559 O ARG 410 40.900 3.901 44.053 1.00 41.78 ATOM 1560 N LYS 411 41.026 6.140 44.325 1.00 52.99 1561 CA LYS 411 **ATOM** 42.109 6.141 45.298 1.00 58.32 **ATOM** 1562 CB LYS 411 41.565 5.956 46.731 1.00 64.99 40.660 4.763 46.977 1.00 70.48 **ATOM** 1563 CG LYS 411 1564 CD LYS 411 ATOM 40.034 4.866 48.364 1.00 77.18 **ATOM** 1565 CE LYS 411 39.053 3.732 48.625 1.00 84.30 ATOM 1566 NZ LYS 411 38.392 3.865 49.958 1.00 86.48 1567 C LYS 411 **ATOM** 43.238 5.163 45.000 1.00 56.66 1568 O LYS ATOM 411 43.329 4.075 45.575 1.00 55.47 **ATOM** 1569 N HIS 412 44.091 5.582 44.070 1.00 54.67 1570 CA HIS **ATOM** 412 45.266 4.823 43.657 1.00 48.67 **ATOM** 1571 CB HIS 412 45.878 5.442 42.393 1.00 43.14 1572 CG HIS ATOM 412 45.073 5.218 41.156 1.00 41.36 **ATOM** 1573 CD2 HIS 412 44.084 5.952 40.584 1.00 35.44 **ATOM** 1574 ND1 HIS 412 45.220 4.093 40.364 1.00 38.19 1575 CE1 HIS **ATOM** 412 44.357 4.150 39.363 1.00 34.75 1576 NE2 HIS 412 ATOM 43.659 5.263 39.474 1.00 35.52 **ATOM** 1577 C HIS 412 46.264 4.932 44.793 1.00 46.35 **ATOM** 1578 O HIS 412 46.326 5.951 45.479 1.00 42.73 **ATOM** 1579 N HIS 413 47.049 3.883 44.993 1.00 48.92 ATOM 1580 CA HIS 413 48.040 3.903 46.052 1.00 53.15 **ATOM** 1581 CB HIS 413 48.148 2.515 46.688 1.00 55.27 1582 CG HIS **ATOM** 46.843 2.015 47.238 1.00 58.77 413 ATOM 1583 CD2 HIS 413 46.138 0.892 46.977 1.00 61.65 ATOM 1584 ND1 HIS 413 46.108 2.726 48.161 1.00 60.31 **ATOM** 1585 CE1 HIS 413 45.003 2.061 48.445 1.00 63.01 **ATOM** 1586 NE2 HIS 413 . 44.993 0.942 47.743 1.00 62.93 ATOM 1587 C HIS 413 49.359 4.364 45.456 1.00 53.19 **ATOM** 1588 O HIS 413 50.335 3.617 45.390 1.00 54.93 **ATOM** 1589 N VAL 414 49.343 5.612 44.999 1.00 53.77 ATOM 1590 CA VAL 414 50.487 6.282 44.389 1.00 51.06 **ATOM** 1591 CB VAL 414 50.374 6.305 42.838 1.00 51.49 ATOM 1592 CG1 VAL 414 51.603 6.958 42.231 1.00 45.22 **ATOM** 1593 CG2 VAL 414 50.210 4.891 42.304 1.00 52.67 **ATOM** 1594 C VAL 414 50.444 7.724 44.894 1.00 54.28

ATOM 1595 O VAL 414 8.401 44.774 1.00 55.49 49.418 ATOM 1596 N THR 415 51.547 8.190 45.467 1.00 56.28 **ATOM** 1597 CA THR 415 51.610 9.550 45.986 1.00 57.83 **ATOM** 1598 CB THR 415 52.874 9.756 46.858 1.00 59.64 1599 OG1 THR 415 **ATOM** 52.922 11.115 47.311 1.00 66.69 ATOM 1600 CG2 THR 415 54.137 9.436 46.067 1.00 59.42 **ATOM** 1601 C THR 415 51.599 10.577 44.855 1.00 56.98 **ATOM** 1602 O THR 415 52.176 10.345 43.789 1.00 55.70 ATOM 1603 N HIS 416 50.936 11.707 45.093 1.00 57.44 1604 CA HIS ATOM 416 50.835 12.786 44.108 1.00 57.34 ATOM 1605 CB HIS 52.207 13.425 43.875 1.00 61.35 416 ATOM 1606 CG HIS 416 52.860 13.940 45.123 1.00 69.78 1607 CD2 HIS ATOM 416 54.049 13.633 45.695 1.00 71.42 1608 ND1 HIS **ATOM** 416 52.283 14.901 45.922 1.00 72.49 ATOM 1609 CE1 HIS 416 53.087 15.165 46.938 1.00 75.50 **ATOM** 1610 NE2 HIS 416 54.165 14.410 46.819 1.00 73.91 ATOM 1611 C HIS 416 50.301 12.260 42.773 1.00 53.79 ATOM 1612 O HIS 416 50.769 12.667 41.710 1.00 52.81 **ATOM** 1613 N PHE 417 49.318 11.366 42.824 1.00 48.05 ATOM 1614 CA PHE 48.769 10.784 41.610 1.00 47.99 417 ATOM 1615 CB PHE 417 47.652 9.799 41.940 1.00 46.11 **ATOM** 1616 CG PHE 417 47.314 8.868 40.791 1.00 44.27 ATOM 1617 CD1 PHE 417 48.155 7.796 40.481 1.00 41.79 ATOM 1618 CD2 PHE 417 46.179 9.091 40.003 1.00 40.23 **ATOM** 1619 CE1 PHE 417 47.872 6.936 39.386 1.00 44.30 ATOM 1620 CE2 PHE 45.874 8.248 38.907 1.00 36.80 417 **ATOM** 1621 CZ PHE 417 46.725 7.167 38.595 1.00 40.69 **ATOM** 1622 C PHE 48.227 11.824 40.625 1.00 46.69 417 **ATOM** 1623 O PHE 417 48.551 11.787 39.436 1.00 43.35 **ATOM** 1624 N TRP 418 47.410 12.746 41.124 1.00 45.14 **ATOM** 1625 CA TRP 418 46.821 13.775 40.276 1.00 44.89 **ATOM** 1626 CB TRP 418 45.808 14.604 41.077 1.00 42.24 **ATOM** 1627 CG TRP 418 45.096 15.646 40.259 1.00 47.11 **ATOM** 1628 CD2 TRP 418 44.186 15.417 39.159 1.00 46.98 ATOM 1629 CE2 TRP 418 43.786 16.678 38.676 1.00 48.94 ATOM 1630 CE3 TRP 43.676 14.261 38.548 1.00 45.23 418 **ATOM** 1631 CD1 TRP 418 45.204 17.003 40.387 1.00 46.24 **ATOM** 1632 NE1 TRP 418 44.425 17.637 39.448 1.00 50.63 **ATOM** 1633 CZ2 TRP 418 42.891 16.839 37.598 1.00 45.46 **ATOM** 1634 CZ3 TRP 418 42.780 14.411 37.468 1.00 44.50 1635 CH2 TRP 418 **ATOM** 42.403 15.696 37.009 1.00 47.55 **ATOM** 1636 C TRP 418 47.862 14.676 39.598 1.00 43.88 **ATOM** 1637 O TRP 418 47.834 14.842 38.383 1.00 43.17 **ATOM** 1638 N PRO 419 48.788 15.281 40.369 1.00 43.55 **ATOM** 1639 CD PRO 419 49.006 15.290 41.826 1.00 41.52 ATOM 1640 CA PRO 419 49.787 16.135 39.725 1.00 41.48

1641 CB PRO 419 ATOM 50.626 16.627 40.912 1.00 39.21 **ATOM** 1642 CG PRO 419 49.593 16.667 42.017 1.00 39.25 ATOM 1643 C PRO 419 50.616 15.363 38.701 1.00 36.28 ATOM 1644 O PRO 419 50.940 15.882 37.638 1.00 37.08 1645 N LYS **ATOM** 420 50.959 14.124 39.033 1.00 35.96 **ATOM** 1646 CA LYS 420 51.742 13.281 38.132 1.00 40.82 **ATOM** 1647 CB LYS 420 52.094 11.945 38.792 1.00 40.78 ATOM 1648 CG LYS 420 53.086 12.046 39.933 1.00 48.62 ATOM 1649 CD LYS 420 53.391 10.668 40.497 1.00 55.12 **ATOM** 1650 CE LYS 420 54.395 10.741 41.635 1.00 53.26 1651 NZ LYS ATOM 420 54.719 9.388 42.152 1.00 52.69 ATOM 1652 C LYS 420 50.957 13.005 36.860 1.00 40.29 **ATOM** 1653 O LYS 420 51.516 12.989 35.764 1.00 39.66 **ATOM** 1654 N LEU 421 49.658 12.786 37.023 1.00 38.33 ATOM 1655 CA LEU 421 48,784 12.507 35.903 1.00 37.60 **ATOM** 1656 CB LEU 421 47.417 12.074 36.428 1.00 43.66 ATOM 1657 CG LEU 46.386 11.479 35.474 1.00 46.50 421 ATOM 1658 CD1 LEU 421 46.946 10.253 34.770 1.00 45.15 1659 CD2 LEU 45.154 11.107 36.279 1.00 51.31 **ATOM** 421 **ATOM** 1660 C LEU 421 48.661 13.747 35.014 1.00 39.59 **ATOM** 1661 O LEU 421 48.599 13.638 33.791 1.00 40.66 **ATOM** 1662 N LEU 422 48.642 14.928 35.623 1.00 39.57 **ATOM** 1663 CA LEU 422 48.545 16.170 34.867 1.00 38.63 ATOM 1664 CB LEU 422 48.313 17.357 35.802 1.00 41.79 **ATOM** 1665 CG LEU 422 46.996 17.407 36.581 1.00 42.74 ATOM 1666 CD1 LEU 422 47.010 18.606 37.515 1.00 42.89 **ATOM** 1667 CD2 LEU 422 45.823 17.494 35.628 1.00 39.27 ATOM 1668 C LEU 49.808 16.410 34.039 1.00 40.47 422 **ATOM** 1669 O LEU 422 49.747 17.029 32.979 1.00 47.83 **ATOM** 1670 N MET 423 50.949 15.936 34.519 1.00 34.27 **ATOM** 1671 CA MET 423 52.187 16.103 33.774 1.00 35.25 ATOM 1672 CB MET 423 53.403 15.716 34.622 1.00 32.56 **ATOM** 1673 CG MET 423 53.675 16.654 35.774 1.00 40.70 **ATOM** 1674 SD MET 423 55.226 16.278 36.597 1.00 47.65 423 **ATOM** 1675 CE MET 54.920 14.601 37.163 1.00 47.16 **ATOM** 1676 C MET 423 52.164 15.254 32.502 1.00 35.13 **ATOM** 423 1677 O MET 52.934 15.499 31.570 1.00 29.85 **ATOM** 424 1678 N LYS 51.285 14.252 32.482 1.00 31.56 **ATOM** 1679 CA LYS 424 51.152 13.384 31.316 1.00 32.29 1680 CB LYS **ATOM** 424 50.373 12.115 31.681 1.00 30.56 **ATOM** 1681 CG LYS 424 51.106 11.178 32.631 1.00 30.07 **ATOM** 1682 CD LYS 424 52.248 10.482 31.938 1.00 33.22 **ATOM** 1683 CE LYS 424 53.059 9.593 32.875 1.00 28.75 ATOM 1684 NZ LYS 424 53.868 10.383 33.833 1.00 31.01 **ATOM** 1685 C LYS 424 50.435 14.150 30.197 1.00 29.26 **ATOM** 50.719 13.944 29.030 1.00 30.22 1686 O LYS 424

ATOM 1687 N VAL 425 49.514 15.036 30.573 1.00 23.53 **ATOM** 1688 CA VAL 425 48.792 15.849 29.601 1.00 28.91 **ATOM** 1689 CB VAL 425 47.808 16.829 30.295 1.00 29.44 ATOM 1690 CG1 VAL 425 47.148 17.737 29.273 1.00 28.81 **ATOM** 1691 CG2 VAL 425 46.744 16.049 31.057 1.00 31.22 1692 C. VAL 425 **ATOM** 49.822 16.669 28.831 1.00 32.03 49.771 16.769 27.605 1.00 31.95 **ATOM** 1693 O VAL 425 **ATOM** 1694 N THR 426 50.763 17.247 29.570 1.00 33.61 ATOM 1695 CA THR 426 51.821 18.057 28.995 1.00 30.76 ATOM 1696 CB THR 426 52.678 18.695 30.105 1.00 32.34 **ATOM** 1697 OG1 THR 426 51.842 19.535 30.912 1.00 33.07 ATOM 1698 CG2 THR 426 53.812 19.533 29.514 1.00 25.40 **ATOM** 1699 C THR 52.712 17.225 28.086 1.00 32.53 426 ATOM 1700 O THR 426 53.113 17.686 27.014 1.00 35.19 **ATOM** 1701 N ASP 427 53.022 16.003 28.507 1.00 28.83 ATOM 1702 CA ASP 427 53.858 15.130 27.695 1.00 35.12 **ATOM** 1703 CB ASP 427 54.273 13.880 28.476 1.00 39.14 ATOM 1704 CG ASP 427 55.122 14.212 29.693 1.00 45.80 ATOM 1705 OD1 ASP 427 56.052 15.034 29.556 1.00 41.97 **ATOM** 1706 OD2 ASP 427 54.869 13.642 30.775 1.00 50.06 **ATOM** 1707 C ASP 427 53.124 14.726 26.422 1.00 33.94 **ATOM** 1708 O ASP 427 53.737 14.617 25.362 1.00 38.02 **ATOM** 1709 N LEU 428 51.818 14.512 26.529 1.00 27.15 **ATOM** 1710 CA LEU 428 51.013 14.148 25.373 1.00 29.99 **ATOM** 1711 CB LEU 428 49.602 13.719 25.802 1.00 22.49 **ATOM** 1712 CG LEU 428 49.541 12.285 26.359 1.00 25.54 ATOM 1713 CD1 LEU 428 48.210 12.021 27.037 1.00 20.60 ATOM 1714 CD2 LEU 428 49.785 11.303 25.224 1.00 17.24 **ATOM** 50.947 15.305 24.381 1.00 28.94 1715 C LEU 428 **ATOM** 1716 O LEU 428 50.941 15.088 23.174 1.00 31.26 ATOM 1717 N ARG 429 50.910 16.531 24.887 1.00 27.64 **ATOM** 1718 CA ARG 429 50.877 17.694 24.011 1.00 28.13 ATOM 1719 CB ARG 429 50.584 18.969 24.800 1.00 29.59 **ATOM** 1720 CG ARG 429 49.224 18.980 25.455 1.00 34.85 **ATOM** 1721 CD ARG 429 48.951 20.314 26.118 1.00 47.18 **ATOM** 1722 NE ARG 429 47.657 20.358 26.797 1.00 57.93 **ATOM** 429 1723 CZ ARG 46.473 20.193 26.200 1.00 63.62 ATOM 1724 NH1 ARG 429 46.402 19.972 24.889 1.00 60.71 **ATOM** 1725 NH2 ARG 429 45.356 20.257 26.919 1.00 62.38 **ATOM** 1726 C ARG 429 52.229 17.819 23.304 1.00 29.81 **ATOM** 1727 O ARG 429 52.294 18.209 22.143 1.00 30.81 1728 N MET **ATOM** 430 53.305 17.482 24.008 1.00 29.64 **ATOM** 1729 CA MET 430 54.639 17.545 23.422 1.00 34.72 **ATOM** 1730 CB MET 430 55.716 17.323 24.485 1.00 34.97 ATOM 1731 CG MET 430 55.864 18.480 25.451 1.00 45.34 1732 SD MET ATOM 430 56.162 20.050 24.596 1.00 52.55

ATOM 1733 CE MET 430 57.598 19.639 23.589 1.00 55.56 **ATOM** 1734 C MET 430 54.778 16.500 22.325 1.00 34.01 **ATOM** 1735 O MET 430 55.440 16.733 21.318 1.00 37.29 1736 N ILE 431 **ATOM** 54.161 15.340 22.533 1.00 29.99 **ATOM** 1737 CA ILE 431 54.197 14.279 21.545 1.00 28.82 1738 CB ILE **ATOM** 431 53.523 12.984 22.095 1.00 27.39 ATOM 1739 CG2 ILE 431 53.260 11.989 20.956 1.00 23.87 ATOM 1740 CG1 ILE 431 54.414 12.386 23.201 1.00 25.56 ATOM 1741 CD1 ILE 431 53.850 11.155 23.896 1.00 17.29 **ATOM** 1742 C ILE 431 53.450 14.785 20.301 1.00 29.49 **ATOM** 1743 O ILE 431 53.908 14.603 19.174 1.00 24.19 **ATOM** 1744 N GLY 432 52.311 15.435 20.524 1.00 25.25 1745 CA GLY 432 **ATOM** 51.542 15.971 19.419 1.00 30.38 ATOM 1746 C GLY 432 52.334 16.997 18.614 1.00 32.75 **ATOM** 1747 O GLY 432 52.410 16.895 17.387 1.00 36.38 **ATOM** 1748 N ALA 433 52.930 17.974 19.294 1.00 26.77 ATOM 1749 CA ALA 433 53.711 19.012 18.625 1.00 26.48 **ATOM** 1750 CB ALA 433 54.182 20.047 19.631 1.00 19.90 **ATOM** 1751 C ALA 433 54.902 18.407 17.890 1.00 30.73 ATOM 1752 O ALA 433 55.207 18.787 16.760 1.00 31.60 1753 N CYS **ATOM** 434 55.582 17.467 18.537 1.00 33.22 1754 CA CYS **ATOM** 434 56.728 16.801 17.914 1.00 34.34 1755 CB CYS ATOM 434 57.339 15.808 18.895 1.00 35.20 **ATOM** 1756 SG CYS 434 59.191 15.745 18.798 1.00 54.48 **ATOM** 1757 C CYS 434 56.313 16.052 16.636 1.00 34.09 **ATOM** 1758 O CYS 434 57.095 15.937 15.679 1.00 34.89 ATOM 1759 N HIS 435 55.088 15.545 16.642 1.00 34.30 1760 CA HIS **ATOM** 435 54.570 14.818 15.501 1.00 35.44 ATOM 1761 CB HIS 435 53.296 14.061 15.886 1.00 31.76 ATOM 1762 CG HIS 435 52.587 13.469 14.715 1.00 32.03 **ATOM** 1763 CD2 HIS 435 52.735 12.277 14.092 1.00 28.61 1764 ND1 HIS **ATOM** 435 51.665 14.177 13.970 1.00 28.48 **ATOM** 1765 CE1 HIS 435 51.284 13.453 12.941 1.00 33.27 ATOM 1766 NE2 HIS 435 51.920 12.284 12.985 1.00 31.57 1767 C HIS 435 **ATOM** 54.311 15.750 14.319 1.00 32.74 1768 O HIS **ATOM** 435 54.504 15.363 13.175 1.00 32.87 1769 N ALA 436 ATOM 53.881 16.975 14.608 1.00 31.01 **ATOM** 1770 CA ALA 436 53.628 17.966 13.571 1.00 29.91 **ATOM** 1771 CB ALA 436 53.221 19.290 14.197 1.00 21.23 **ATOM** 1772 C ALA 436 54.911 18.135 12.769 1.00 33.86 **ATOM** 1773 O ALA 436 54.892 18.128 11.541 1.00 36.10 **ATOM** 1774 N SER 437 56.030 18.266 13.483 1.00 35.19 1775 CA SER 437 **ATOM** 57.344 18.426 12.871 1.00 33.03 1776 CB SER 437 **ATOM** 58.389 18.720 13.941 1.00 35.31 **ATOM** 1777 OG SER 437 59.681 18.782 13.373 1.00 44.99 ATOM 1778 C SER 437 57.758 17.178 12.100 1.00 38.39

ATOM 1779 O SER 437 58.374 17.269 11.034 1.00 37.54 ATOM 1780 N ARG 438 57.427 16.012 12.642 1.00 37.32 1781 CA ARG **ATOM** 438 57.762 14.754 11.992 1.00 39.30 **ATOM** 1782 CB ARG 438 57.517 13.572 12.941 1.00 42.97 **ATOM** 1783 CG ARG 438 58.542 13.436 14.059 1.00 41.72 **ATOM** 1784 CD ARG 438 59.926 13.212 13.484 1.00 45.23 **ATOM** 1785 NE ARG 438 59.961 12.050 12.601 1.00 45.66 1786 CZ ARG 60.935 11.804 11.731 1.00 49.71 ATOM 438 ATOM 1787 NH1 ARG 438 61.961 12.641 11.627 1.00 50.91 **ATOM** 1788 NH2 ARG 438 60.885 10.727 10.960 1.00 46.86 **ATOM** 1789 C ARG 438 56.939 14.565 10.725 1.00 42.37 **ATOM** 1790 O ARG 438 57.311 13.794 9.841 1.00 40.58 ATOM 1791 N PHE 439 55.816 15.269 10.645 1.00 42.25 1792 CA PHE 439 54.957 15.170 9.479 1.00 42.81 ATOM **ATOM** 1793 CB PHE 439 53.593 15.790 9.771 1.00 42.18 1794 CG PHE **ATOM** 439 52.594 15.597 8.656 1.00 42.48 ATOM 1795 CD1 PHE 439 52.173 14.312 8.295 1.00 47.09 439 **ATOM** 1796 CD2 PHE 52.086 16.696 7.961 1.00 39.76 1797 CE1 PHE 439 **ATOM** 51.256 14.110 7.234 1.00 49.17 1798 CE2 PHE 439 **ATOM** 51.174 16.524 6.896 1.00 45.10 **ATOM** 1799 CZ PHE 439 50.751 15.225 6.532 1.00 46.36 **ATOM** 1800 C PHE 439 55.626 15.905 8.322 1.00 44.79 7.181 1.00 40.26 **ATOM** 1801 O PHE 439 55.596 15.444 440 **ATOM** 1802 N LEU 56.236 17.049 8.629 1.00 42.77 1803 CA LEU **ATOM** 440 56.927 17.839 7.621 1.00 42.96 1804 CB LEU 440 **ATOM** 57.421 19.156 8.216 1.00 37.19 1805 CG LEU 440 **ATOM** 56.348 20.117 8.725 1.00 36.97 **ATOM** 1806 CD1 LEU 440 57.020 21.338 9.321 1.00 33.65 **ATOM** 1807 CD2 LEU 440 55.411 20.519 7.572 1.00 35.42 1808 C LEU 440 **ATOM** 58.106 17.063 7.053 1.00 45.47 **ATOM** 1809 O LEU 440 58.421 17.191 5.876 1.00 52.48 ATOM 1810 N HIS 441 58.760 16.266 7.890 1.00 49.15 **ATOM** 1811 CA HIS 441 59.893 15.473 7.435 1.00 54.76 **ATOM** 1812 CB HIS 441 60.723 14.964 8.624 1.00 56.68 **ATOM** 1813 CG HIS 441 61.515 16.026 9.323 1.00 62.73 ATOM 1814 CD2 HIS 441 62.851 16.166 9.508 1.00 65.73 **ATOM** 1815 ND1 HIS 441 60.929 17.098 9.966 1.00 66.01 **ATOM** 441 1816 CE1 HIS 61.871 17.845 10.518 1.00 65.55 **ATOM** 1817 NE2 HIS 441 63.044 17.306 10.258 1.00 60.09 **ATOM** 1818 C HIS 441 59.417 14.292 6.589 1.00 55.93 **ATOM** 1819 O HIS 441 60.084 13.908 5.630 1.00 57.33 1820 N MET **ATOM** 442 58.271 13.716 6.948 1.00 57.81 **ATOM** 1821 CA MET 442 6.203 1.00 59.11 57.712 12.585 **ATOM** 1822 CB MET 442 56.562 11.924 6.978 1.00 55.93 **ATOM** 1823 CG MET 442 56.961 11.246 8.276 1.00 58.52 1824 SD MET 442 55.564 10.420 9.105 1.00 60.99 ATOM

ATOM 1825 CE MET 442 54.430 11.779 9.350 1.00 52.61 ATOM 1826 C **MET** 442 57.178 13.065 4.854 1.00 60.31 **ATOM** 1827 O **MET** 442 57.279 12.369 3.846 1.00 58.18 **ATOM** 1828 N LYS 443 56.608 14.266 4.863 1.00 61.45 1829 CA LYS ATOM 443 56.038 14.871 3.669 1.00 64.90 **ATOM** 1830 CB LYS 443 55.434 16.232 4.035 1.00 64.40 **ATOM** 1831 CG LYS 54.589 16.872 2.945 1.00 69.12 443 **ATOM** 1832 CD LYS 443 54.064 18.250 3.363 1.00 71.14 **ATOM** 1833 CE LYS 443 53.138 18.183 4.575 1.00 73.43 ATOM 1834 NZ LYS 52.668 19.534 5.015 1.00 67.97 443 **ATOM** 1835 C LYS 443 57.112 15.030 2.585 1.00 67.29 **ATOM** 1836 O LYS 443 56.800 15.218 1.406 1.00 67.90 1837 N VAL 444 **ATOM** 58.373 14.941 2.996 1.00 66.57 1838 CA VAL ATOM 444 59.501 15.064 2.078 1.00 64.76 ATOM 1839 CB VAL 444 60.618 15.940 2.693 1.00 62.76 **ATOM** 1840 CG1 VAL 444 61.767 16.092 1.712 1.00 64.00 1841 CG2 VAL 444 ATOM 60.062 17.301 3.072 1.00 59.27 **ATOM** 1842 C VAL 444 60.091 13.693 1.744 1.00 68.61 **ATOM** 1843 O VAL 444 60.145 13.294 0.577 1.00 70.60 1844 N GLU 445 **ATOM** 60.520 12.972 2.775 1.00 70.71 **ATOM** 1845 CA GLU 445 61.129 11.653 2.609 1.00 71.45 **ATOM** 1846 CB GLU 445 61.808 11.233 3.916 1.00 72.36 **ATOM** 1847 C GLU 445 60.181 10.547 2.148 1.00 71.46 1848 O GLU **ATOM** 445 60.588 9.390 2.042 1.00 73.02 1849 N CYS 446 **ATOM** 58.925 10.895 1.871 1.00 71.12 **ATOM** 1850 CA CYS 446 57.945 9.901 1.419 1.00 70.83 **ATOM** 1851 CB CYS 446 57.031 9.485 2.581 1.00 71.05 **ATOM** 1852 SG CYS 446 57.845 8.593 3.925 1.00 72.83 **ATOM** 1853 C CYS 446 57.081 10.390 0.261 1.00 71.91 1854 O CYS **ATOM** 446 56.776 11.582 0.155 1.00 72.06 **ATOM** 1855 N PRO 447 56.673 9.470 -0.635 1.00 73.12 1856 CD PRO 447 56.967 8.026 -0.671 1.00 72.88 **ATOM ATOM** 1857 CA PRO 447 55.837 9.825 -1.784 1.00 74.22 **ATOM** 1858 CB PRO 447 55.717 8.500 -2.537 1.00 72.98 **ATOM** 1859 CG PRO 447 57.015 7.790 -2.161 1.00 74.77 447 **ATOM** 1860 C PRO 54.479 10.343 -1.330 1.00 75.94 **ATOM** 1861 O PRO 447 53.754 9.652 -0.616 1.00 76.67 1862 N THR 448 54.145 11.558 -1.755 1.00 76.91 ATOM **ATOM** 1863 CA THR 448 52.879 12.197 -1.403 1.00 78.24 1864 CB THR 448 52.647 13.459 -2.261 1.00 81.33 **ATOM ATOM** 1865 OG1 THR 448 52.552 13.087 -3.643 1.00 84.46 53.802 14.444 -2.089 1.00 83.51 **ATOM** 1866 CG2 THR 448 51.676 11.270 -1.580 1.00 77.42 **ATOM** 1867 C THR 448 **ATOM** 1868 O THR 448 50.662 11.413 -0.894 1.00 77.65 1869 N GLU 449 51.795 10.319 -2.502 1.00 76.29 **ATOM ATOM** 1870 CA GLU 449 50.720 9.375 -2.783 1.00 75.03

ATOM 1871 CB GLU 449 51.048 8.572 -4.043 1.00 74.62 1872 C GLU **ATOM** 449 50.445 8.421 -1.622 1.00 73.49 1873 O ATOM GLU 449 49.310 7.973 -1.442 1.00 70.24 ATOM 1874 N LEU 450 51.477 8.113 -0.840 1.00 70.80 1875 CA LEU **ATOM** 450 51.327 7.194 0.285 1.00 68.82 ATOM 1876 CB LEU 450 52.693 6.644 0.705 1.00 71.91 ATOM 1877 CG LEU 450 53.428 5.795 -0.336 1.00 76.62 **ATOM** 1878 CD1 LEU 450 54.799 5.414 0.195 1.00 77.95 **ATOM** 1879 CD2 LEU 450 52.617 4.546 -0.662 1.00 76.46 **ATOM** 1880 C LEU 450 50.636 7.818 1.492 1.00 66.22 **ATOM** 1881 O LEU 450 50.501 7.181 2.540 1.00 66.01 **ATOM** 1882 N PHE 451 50.189 9.060 1.342 1.00 61.96 1883 CA PHE **ATOM** 451 49.513 9.750 2.428 1.00 58.44 **ATOM** 1884 CB PHE 451 50.006 11.204 2.528 1.00 61.34 **ATOM** 1885 CG PHE 451 51.466 11.343 2.923 1.00 63.02 **ATOM** 1886 CD1 PHE 451 52.488 10.888 2.077 1.00 62.92 **ATOM** 1887 CD2 PHE 451 51.812 11.932 4.146 1.00 63.07 ATOM 1888 CE1 PHE 451 53.855 11.029 2.437 1.00 65.12 **ATOM** 1889 CE2 PHE 451 53.167 12.085 4.531 1.00 64.66 **ATOM** 1890 CZ PHE 451 54.195 11.628 3.673 1.00 67.12 **ATOM** 1891 C PHE 451 48.005 9.756 2.219 1.00 56.41 ATOM 1892 O PHE 451 47.501 10.471 1.350 1.00 56.56 **ATOM** 1893 N PRO 452 47.260 8.954 3.009 1.00 53.28 **ATOM** 1894 CD PRO 452 47.678 8.027 4.076 1.00 50.46 **ATOM** 1895 CA PRO 452 45.797 8.910 2.866 1.00 50.26 **ATOM** 1896 CB PRO 452 45.388 7.976 4.000 1.00 49.19 **ATOM** 1897 CG PRO 452 46.558 7.010 4.039 1.00 45.89 **ATOM** 1898 C PRO 452 45.183 10.305 2.974 1.00 49.62 1899 O PRO **ATOM** 452 45.727 11.176 3.644 1.00 52.35 **ATOM** 1900 N PRO 453 44.034 10.530 2.313 1.00 51.50 **ATOM** 1901 CD PRO 453 43.257 9.585 1.494 1.00 49.66 ATOM 1902 CA PRO 453 43.354 11.830 2.335 1.00 50.89 **ATOM** 1903 CB PRO 453 42.101 11.559 1.506 1.00 51.49 1904 CG PRO 453 **ATOM** 42.600 10.524 0.521 1.00 50.82 **ATOM** 1905 C PRO 453 43.030 12.405 3,706 1.00 50.99 ATOM 1906 O PRO 453 43.264 13.588 3.953 1.00 54.17 **ATOM** 1907 N LEU 454 42.479 11.576 4.592 1.00 51.21 **ATOM** 1908 CA LEU 454 42.112 12.034 5.936 1.00 47.17 ATOM 1909 CB LEU 454 41.305 10.951 6.660 1.00 44.44 **ATOM** 1910 CG LEU 454 40.748 11.283 8.050 1.00 41.33 **ATOM** 1911 CD1 LEU 454 39.838 12.504 7.978 1.00 35.93 39.986 10.072 8.587 1.00 34.79 ATOM 1912 CD2 LEU 454 **ATOM** 1913 C LEU 454 43.363 12.380 6.733 1.00 42.25 **ATOM** 1914 O LEU 454 43.387 13.357 7.475 1.00 40.82 **ATOM** 1915 N PHE 455 44.399 11.567 6.565 1.00 39.29 **ATOM** 1916 CA PHE 455 45.674 11.774 7.240 1.00 41.81

ATOM 1917 CB PHE 455 46.655 10.679 6.802 1.00 47.22 1918 CG PHE ATOM 455 48.045 10.800 7.407 1.00 56.97 **ATOM** 1919 CD1 PHE 455 48.220 10.990 8.785 1.00 57.23 **ATOM** 1920 CD2 PHE 455 49.180 10.645 6.597 1.00 59.40 1921 CE1 PHE **ATOM** 455 49.522 11.030 9.362 1.00 56.58 **ATOM** 1922 CE2 PHE 455 50.487 10.682 7.149 1.00 61.80 **ATOM** 1923 CZ PHE 455 50.656 10.870 8.541 1.00 59.94 **ATOM** 1924 C PHE 455 46.203 13.161 6.892 1.00 45.12 ATOM 1925 O PHE 46.558 13.944 7.779 1.00 39.95 455 **ATOM** 1926 N LEU 456 46.236 13.471 5.592 1.00 43.92 **ATOM** 1927 CA LEU 456 46.704 14.767 5.123 1.00 44.08 1928 CB LEU **ATOM** 456 46.748 14.795 3.593 1.00 50.20 **ATOM** 1929 CG LEU 456 47.796 13.921 2.903 1.00 55.79 1930 CD1 LEU ATOM 456 47.527 13.869 1.408 1.00 54.70 **ATOM** 1931 CD2 LEU 456 49.187 14.473 3.193 1.00 53.01 **ATOM** 1932 C LEU 456 45.782 15.871 5.616 1.00 44.65 1933 O LEU ATOM 456 46.219 16.987 5.887 1.00 45.93 **ATOM** 1934 N GLU 457 44.500 15.549 5.726 1.00 44.56 **ATOM** 1935 CA GLU 457 43.498 16.504 6.175 1.00 46.37 1936 CB GLU **ATOM** 457 42.138 15.854 6.133 1.00 50.16 **ATOM** 1937 C **GLU 457** 43.759 17.039 7.579 1.00 43.60 **ATOM** 1938 O GLU 457 43.867 18.245 7.795 1.00 42.69 **ATOM** 1939 N VAL 458 43.847 16.117 8.528 1.00 43.21 **ATOM** 1940 CA VAL 458 44.064 16.446 9.930 1.00 44.98 **ATOM** 1941 CB VAL 458 44.020 15.159 10.802 1.00 44.83 **ATOM** 1942 CG1 VAL 458 44.180 15.510 12.277 1.00 49.72 **ATOM** 1943 CG2 VAL 458 42.708 14.427 10.567 1.00 40.89 **ATOM** 1944 C VAL 458 45.368 17.178 10.209 1.00 42.72 1945 O VAL 458 **ATOM** 45.393 18.139 10.974 1.00 42.88 1946 N PHE **ATOM** 459 46.451 16.743 9.574 1.00 44.53 **ATOM** 1947 CA PHE 459 47.741 17.366 9.823 1.00 48.18 1948 CB PHE 459 ATOM 48.784 16.269 10.064 1.00 43.60 **ATOM** 1949 CG PHE 459 48.374 15.276 11.133 1.00 40.79 47.835 14.032 10.783 1.00 41.01 **ATOM** 1950 CD1 PHE 459 **ATOM** 1951 CD2 PHE 459 48.471 15.613 12.492 1.00 39.48 **ATOM** 1952 CE1 PHE 459 47.387 13.118 11.776 1.00 40.62 **ATOM** 1953 CE2 PHE 459 48.032 14.715 13.506 1.00 36.87 1954 CZ PHE **ATOM** 459 47.489 13.463 13.146 1.00 36.39 **ATOM** 1955 C PHE 459 48.234 18.348 8.763 1.00 52.71 459 **ATOM** 1956 O PHE 49.336 18.878 8.877 1.00 51.34 **ATOM** 1957 N GLU 460 47.397 18.594 7.752 1.00 59.56 **ATOM** 1958 CA GLU 460 47.695 19.509 6.647 1.00 66.14 **ATOM** 1959 CB GLU 460 47.818 20.944 7.158 1.00 67.76 **ATOM** 1960 CG GLU 460 46.536 21.511 7.724 1.00 78.99 1961 CD GLU 46.680 22.965 8.116 1.00 86.08 **ATOM** 460 ATOM 1962 OE1 GLU 460 47.014 23.786 7.237 1.00 87.62

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ATOM	1963	OE2 GL	U 460	46.40	60 23.2	289 9.3	301 1.00 91.63	,
ATOM	1964	C GLU	J 460	48.940			6 1.00 69.17	
ATOM	1965	O GLU	460	48.78	4 18.75	59 4.66	0 1.00 69.49	·
ATOM	1966	OXT GL	U 460	50.0	57 19.2	298 6.3	379 1.00 76.70)
ATOM	1967	C1 TRI	1	47.283	4.313	16.972	1.00 44.70	
ATOM	1968	C2 TRI	1	51.052	6.807	13.814	1.00 34.01	
ATOM		C3 TRI	1.	47.289	4.043	15.500	1.00 37.90	
ATOM		C4 TRI	1.	51.936	6.615	12.728	1.00 33.38	
ATOM		C5 TRI	1	48.462	4.501	14.746	1.00 46.53	
ATOM	1972		1	52.294	7.653	11.847	1.00 42.90	
ATOM		C7 TRI	1	49.577	5.179	15.334	1.00 34.63	
ATOM		C8 TRI	1	51.717	9.015	12.071	1.00 38.34	
ATOM		C9 TRI	1	49.492	5.383	16.723	1.00 43.89	
ATOM		C10 TRI	1	50.779		13.172	1.00 40.43	
ATOM		C11 TRI	1	48.354		17.533	1.00 41.82	•
ATOM		C12 TRI	1	50.449		14.055	1.00 35.64	
ATOM		C13 TRI	1	46.287		17.959	1.00 36.78	
ATOM		C15 TRI	1	44.825		17.865	1.00 40.69	
ATOM		1 TRI	-				1.00 40.26	
ATOM		2 TRI	1				1.00 46.70	•
ATOM	1983 I		1				1.00 36.54	
ATOM		O3 TRI	1			17.329	1.00 54.78	
ATOM		D2 TRI	1	50.831		14.667	1.00 28.44	
ATOM		OI TRI	1	52.207			1.00 43.65	
ATOM	1987		1	44.021		18.352	1.00 42.95	
ATOM		S CAC	501	60.548			1.00 65.97	AS
ATOM		S CAC	502			16.796		AS
ATOM	3 AS		503	29.889	28.698			AS
ATOM ATOM	4 AS 5 O	S CAC HOH	504	33.547	24.203	8.880	1.00100.00	AS
ATOM	6 0	НОН	505 506	42.365	8.872	4.597	1.00 53.88	HOH
ATOM	7 0	НОН	507	33.545 37.040				HOH
ATOM	8 0	НОН	508	44.105			1.00 61.87 1.00 40.68	HOH
ATOM	9 0	НОН	509				1.00 40.08	HOH HOH
ATOM	10 O	НОН	510				1.00 55.36	НОН
ATOM	11 0	НОН	511				1.00 33.30	НОН
ATOM	12 0	НОН	512				1.00 55.42	НОН
ATOM	13 O	НОН	513				1.00 58.30	HOH
ATOM	14 0	НОН	514				1.00 50.35	HOH
ATOM	15 O	НОН	515	37.467			1.00 30.33	НОН
ATOM	16 O		516				1.00 57.40	НОН
ATOM	17 O	НОН	517				1.00 63.46	НОН
ATOM	18 O	НОН	518	33.622		47.570	1.00 53.40	НОН
ATOM	19 O	НОН	519	64.787		11.882	1.00 55.07	НОН
ATOM	20 O	НОН	520				1.00 61.70	НОН
ATOM	21 O	НОН	521				1.00 40.50	НОН
				17.007	J. 172	JU.J-J	1.00 10.00	11011

ATOM	22 (нон с	522	43.786	-0.987	26.878	1.00 52.16	НОН
ATOM	23 (HOH C	523	41.604	2.361	26.985		НОН
ATOM	24 (нон С	524	54.405	6.361	39.795	1.00 56.56	НОН
ATOM	25 (нон с	525	46.088	0.770	33.095	1.00 74.24	НОН
ATOM	26 (HOH C	526	50.481	16.245	15.314	1.00 28.99	НОН
ATOM	27 (HOH	527	59.788	14.863	21.416	1.00 50.02	НОН
ATOM	28 (HOH	528	49.282	19.490	32.191	1.00 41.61	НОН
ATOM	29 (HOH (529	56.683	10.961	26.733	1.00 34.20	НОН
ATOM	30 C	HOH (530	56.701	9.852	30.561	1.00 51.24	НОН
ATOM	31 C	HOH (531	26.487	13.273	30.591	1.00 43.94	HOH
ATOM	32 C	HOH (532	27.019	25.052	28.330	1.00 54.97	HOH
ATOM	33 C	HOH (533	50.689	1.918	29.551	1.00 30.63	HOH
ATOM	34 C	HOH	534	47.867	0.200	31.330	1.00 43.14	HOH
ATOM	35 C	HOH	535	61.434	-0.721	23.218	1.00 49.83	HOH
ATOM	36 C	HOH	536	41.969	20.017	20.894	1.00 27.00	HOH
ATOM	37 C	HOH	537	46.897	16.244	15.992	1.00 31.50	HOH
ATOM	38 O	HOH	538	29.796	16.276	27.000	1.00 38.52	HOH
ATOM	39 O	HOH	539	47.853	23.205	20.217	1.00 44.39	HOH
ATOM	40 O	HOH	540	40.956	24.775	31.717	1.00 50.36	HOH
ATOM	41 O	HOH	541	43.310	1.560	41.912	1.00 43.56	HOH
END								